STIC Search Report
EIC 1700

STIC Database Tracking Number: 111906

TO:	From:
Michael Lavilla Location: REM 5E79 Art Unit : 1775 January 14, 2004 Case Serial Number: 09/890438	Kathleen Fuller Location: EIC 1700 REMSEN 4B28 Phone: 571/272-2505 Kathleen.Fuller@uspto.gov

Search Notes

STIC Search Results Feedback Form

EIC17000

Questions about the scope or the results of the search? Contact ***the EIC searcher or contact*:**

Kathleen Fuller, EIC 1700 Team Leader
571/272-2505 REMSEN 4B28

Voluntary Results Feedback Form

- *I am an examiner in Workgroup:* ☐ *Example: 1713*
- *Relevant prior art **found**, search results used as follows:*
  - ☐ 102 rejection
  - ☐ 103 rejection
  - ☐ Cited as being of interest.
  - ☐ Helped examiner better understand the invention.
  - ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
  (journal articles, conference proceedings, new product announcements etc.)

- *Relevant prior art **not found:***
  - ☐ Results verified the lack of relevant prior art (helped determine patentability).
  - ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to EIC1700 REMSEN 4B28

=> FILE REG
FILE 'REGISTRY' ENTERED AT 11:42:53 ON 14 JAN 2004

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 12 JAN 2004 HIGHEST RN 636984-67-3
DICTIONARY FILE UPDATES: 12 JAN 2004 HIGHEST RN 636984-67-3

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

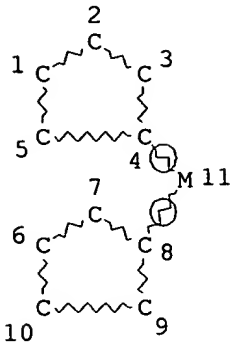
=> FILE HCAPLUS
FILE 'HCAPLUS' ENTERED AT 11:42:57 ON 14 JAN 2004

FILE COVERS 1907 - 14 Jan 2004 VOL 140 ISS 3
FILE LAST UPDATED: 13 Jan 2004 (20040113/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> D QUE L34
L20 STR

structure 1

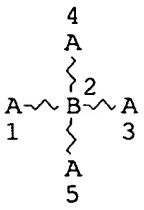


NODE ATTRIBUTES:
NSPEC IS R AT 11
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE
L22 STR 2

3,302 structures from the query



NODE ATTRIBUTES:
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NSPEC IS RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE
L24 SCR 1966 OR 1984 OR 1975
L25 SCR 1921 AND 1965
L26 SCR 1931 AND 1965
L27 SCR 1964 AND 2001
L29 3302 SEA FILE=REGISTRY SSS FUL L20 AND L22 AND (L24 OR L25 OR L26 OR L27)
L30 1647 SEA FILE=HCAPLUS ABB=ON L29
L33 136 SEA FILE=HCAPLUS ABB=ON L30(L)CAT/RL(L)POLYMERI?
L34 26 SEA FILE=HCAPLUS ABB=ON L33 AND CRYSTAL?

26 CA references with utility

=> D L34 ALL 1-26 HITSTR

L34 ANSWER 1 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:331258 HCAPLUS
DN 139:53111
ED Entered STN: 01 May 2003
TI C-H Activation of the Trimethylsilyl-Substituted Cyclopentadienyl Ligand in the "Cation-like" Complex [Cp'''2ZrMe][MeB(C6F5)3] (Cp''' = η5-C5H2-1,2,4-(SiMe3)3)
AU Choukroun, Robert; Wolff, Fabien; Lorber, Christian; Donnadieu, Bruno
CS Laboratoire de Chimie de Coordination, CNRS UPR 8241, Toulouse, 31077, Fr.
SO Organometallics (2003), 22(11), 2245-2248
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 75
OS CASREACT 139:53111
AB The substituted cyclopentadienyl Zr complex [Cp'''2ZrMe2] (1; Cp''' = η5-C5H2-1,2,4-(SiMe3)3) reacts with tris(perfluorophenyl)borane, B(C6F5)3, in pentane to give the two species [Cp'''2ZrMe][MeB(C6F5)3] (2) and [Cp'''(η5-C5H2-2,4-(SiMe3)2-1-η1-SiMe2CH2)Zr][MeB(C6F5)3] (3). Complex 3 was characterized by an x-ray structure determination, showing the C-H activation of a SiMe3 group attached to the cyclopentadienyl ligand. Complexes 2 and 3 could be described, resp., as the active and inactive species which both arise from 1 and B(C6F5)3 in the cationic polymerization of ethylene.
ST zirconocene silyl substituted carbon hydrogen activation borane perfluorophenyl; **crystal** structure zirconocene silyl methylene bridged prepn; mol structure zirconocene silyl methylene bridged
IT Bond
(carbon-hydrogen, activation; C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand in silyl ring-substituted zirconocene derivative)
IT Polymerization catalysts
(cationic, deactivation by cyclopentadienyl ligand degradation; C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand in silyl ring-substituted zirconocene derivative)
IT **Crystal** structure
Molecular structure
(of methylene-bridged zirconocene complex having silyl ring substituents)
IT 172296-04-7
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand in silyl ring-substituted zirconocene polymerization catalyst)
IT **545446-19-3P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand in silyl ring-substituted zirconocene **polymerization** catalyst)
IT 74-85-1, Ethylene, reactions 1109-15-5, Tris(perfluorophenyl)borane
RL: RCT (Reactant); RACT (Reactant or reagent)
(C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand

in silyl ring-substituted zirconocene polymerization catalyst)

IT 9002-88-4P, Polyethylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand in silyl ring-substituted zirconocene polymerization catalyst)

IT 545446-20-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(**crystal** structure, failed as polymerization catalyst; C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand in silyl ring-substituted zirconocene polymerization catalyst)

RE.CNT 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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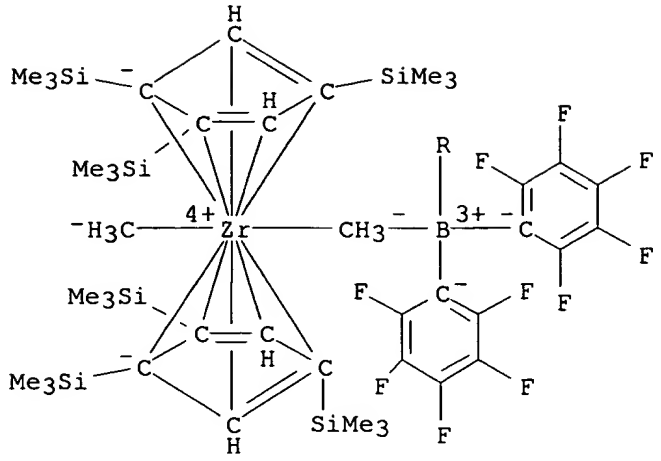
IT **545446-19-3P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(C-H activation of trimethylsilyl-substituted cyclopentadienyl ligand in silyl ring-substituted zirconocene **polymerization** catalyst)

RN 545446-19-3 HCAPLUS

CN Zirconium, μ-methylmethyl[tris(pentafluorophenyl)boron]bis[(1,2,3,4,5-η)-1,2,4-tris(trimethylsilyl)-2,4-cyclopentadien-1-yl]- (9CI) (CA INDEX NAME)

PAGE 1-A



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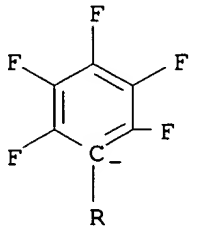

L34 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2003:16277 HCAPLUS
DN 138:221668
ED Entered STN: 09 Jan 2003
TI Ferrocene-Based Olefin Polymerization Catalysts: Activation, Structure, and Intermediates
AU Shafir, Alexandr; Arnold, John
CS Department of Chemistry, University of California, Berkeley, CA, 94720-1460, USA
SO Organometallics (2003), 22(3), 567-575
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-12 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 35, 75
OS CASREACT 138:221668
AB This paper describes abstraction of a benzyl group from the Zr dibenzyl complex 1,1'-Fc(NSiMe3)2ZrBn2 (1) using B(C6F5)3 and [Ph3C][B(C6F5)4] (TB). In both cases, clean formation of the corresponding cationic monobenzyl species LZrBn+ (L = 1,1'-Fc(NSiMe3)22-) was observed by NMR spectroscopy. In the case of [LZrBn][BnB(C6F5)3] (2), an x-ray

crystal structure determination confirmed an η6 coordination of the borate benzyl group to the cationic Zr center. Reaction of this complex with 1 equiv of C2H2 or RCCR (R = Me, Ph) proceeded with rapid single insertion of the olefin or acetylene into the Zr-carbon σ-bond. With ethylene or 2-butyne further insertions occur more slowly and longer chains were obtained upon addition of more monomer. Activation of 1 with TB leads to an active ethylene polymerization catalyst, producing 102 g of PE mmol-1 atm-1 h-1. Compound 2 reacted with CH2Cl2 to form the dimeric [LZrCl2]2, which was characterized **crystallog**.

ST ferrocene zirconium silylamide complex prepn olefin polymn catalyst; **crystal** mol structure ferrocene zirconium silylamide benzylborato complex prepn; zirconium ferrocene silylamide chloro bridged prepn **crystal** mol structure; fluxional rearrangement ferrocene zirconium silylamide benzyl complex prepn

IT **Crystal** structure
Molecular structure
(of ferrocene zirconium silylamide complexes)

IT Polymerization
Polymerization catalysts
(preparation of ferrocene zirconium silylamide complexes as olefin polymerization catalysts)

IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of ferrocene zirconium silylamide complexes as olefin polymerization catalysts)

IT 500772-21-4P 500772-22-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(**crystal** structure; preparation of ferrocene zirconium silylamide complexes as olefin polymerization catalysts)

IT **500772-11-2P**
RL: **CAT (Catalyst use)**; CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(fluxional rearrangement; preparation of ferrocene zirconium silylamide complexes as olefin **polymerization** catalysts)

IT 500772-19-0P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(fluxional rearrangement; preparation of ferrocene zirconium silylamide complexes as olefin polymerization catalysts)

IT 2294-94-2P
RL: BYP (Byproduct); PREP (Preparation)
(preparation of ferrocene zirconium silylamide complexes as olefin polymerization catalysts)

IT 74-85-1, Ethylene, reactions 501-65-5, Diphenylacetylene 503-17-3, 2-Butyne 1109-15-5 2789-88-0, Di-p-tolylacetylene 6921-34-2, Benzylmagnesium chloride" 136040-19-2 337456-29-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of ferrocene zirconium silylamide complexes as olefin polymerization catalysts)

IT 212394-79-1P 500772-09-8P 500772-14-5P 500772-18-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
(preparation of ferrocene zirconium silylamide complexes as olefin polymerization
catalysts)
IT 9002-88-4P, Polyethylene 500772-12-3P 500772-16-7P 500772-20-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of ferrocene zirconium silylamide complexes as olefin polymerization
catalysts)
RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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IT **500772-11-2P**
RL: **CAT (Catalyst use)**; CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)

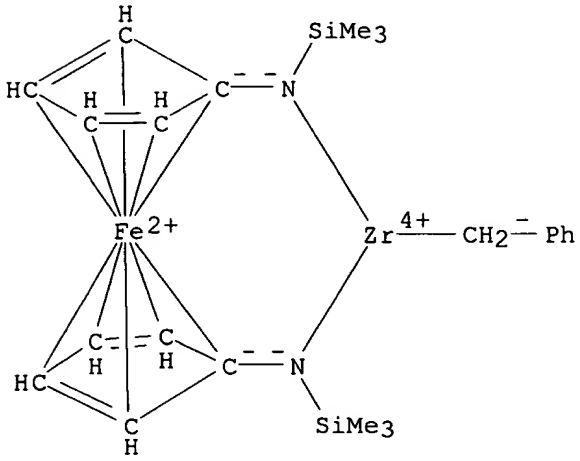
(fluxional rearrangement; preparation of ferrocene zirconium silylamide complexes as olefin **polymerization** catalysts)

RN 500772-11-2 HCAPLUS

CN Zirconium(1+), [1,1'-bis[(trimethylsilyl)amino-κN]ferrocenato(2-)](phenylmethyl)-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

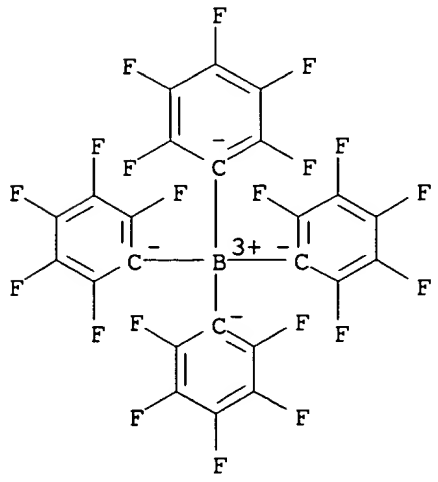
CM 1

CRN 500772-10-1
CMF C23 H33 Fe N2 Si2 Zr
CCI CCS



CM 2

CRN 47855-94-7
CMF C24 B F20
CCI CCS



L34 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:841308 HCAPLUS
DN 138:73599
ED Entered STN: 06 Nov 2002
TI Branching Formation in the Ethylene Polymerization with Meso Ansa Metallocene-Based Catalysts
AU Melillo, Gianluca; Izzo, Lorella; Zinna, Marianna; Tedesco, Consiglia; Oliva, Leone
CS Dipartimento di Chimica, Universita di Salerno, Baronissi, I-84081, Italy
SO Macromolecules (2002), 35(25), 9256-9261
CODEN: MAMOBX; ISSN: 0024-9297
PB American Chemical Society
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67, 75
AB An investigation of the ethylene polymerization with meso ansa metallocenes of group 4 allows clarifying some aspects of the branching formation observed in the polyethylene produced with these catalysts. The meso structure of the zirconocene precursor is more effective in promoting the chain growing isomerization when indenyl ligands bear no substituents. But the same coordinating neighborhood when surrounding the Ti(IV) or Hf(IV) ion gives rise to complexes not effective in the ethyl-branched polyethylene synthesis. On the other hand, several activators in combination with meso-ethylenebis(1-indenyl)Zr(CH3)2 produce catalysts able to polymerize ethylene to ethyl-branched polyethylene. No difference has been detected in the amount of branches with respect to that observed with MAO-activated meso-ethylenebis(1-indenyl)ZrCl2.
ST meso ansa metallocene catalyst branching formation ethylene polymn; polyethylene chain branching metallocene catalyst effect
IT Aluminoxanes
RL: CAT (Catalyst use); USES (Uses)
(Me, cocatalyst, nonmodified and modified; branching formation in ethylene polymerization with meso ansa metallocene-based catalysts)
IT Polymerization
(branching formation in ethylene polymerization with meso ansa metallocene-based catalysts)
IT Polymer chains
(branching; branching formation in ethylene polymerization with meso ansa metallocene-based catalysts)
IT Solvent effect
(on branching formation in ethylene polymerization with meso ansa metallocene-based catalysts)
IT **Crystal** structure
(preparation and **crystal** structure of meso ansa metallocene-based catalysts and branching formation in ethylene polymerization in presence of these catalysts)
IT Metallocenes
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and **crystal** structure of meso ansa metallocene-based catalysts and branching formation in ethylene polymerization in presence of these catalysts)
IT Polymerization catalysts
(preparation of meso ansa metallocene-based catalysts and branching formation in ethylene polymerization in presence of these catalysts)

IT 83417-92-9 148799-45-5 159572-55-1 167254-68-4 367522-39-2
RL: CAT (Catalyst use); USES (Uses)
(branching formation in ethylene polymerization with meso ansa metallocene-based catalysts)
IT 9002-88-4P, Polyethylene
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(branching formation in ethylene polymerization with meso ansa metallocene-based catalysts)
IT 1109-15-5, Tris(pentafluorophenyl)boron
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(cocatalyst and reactant in catalyst preparation; preparation of meso ansa metallocene-based catalysts and branching formation in ethylene polymerization
in presence of these catalysts)
IT 136040-19-2, Triphenylcarbonium tetrakis(pentafluorophenyl)borate
167172-28-3
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst; branching formation in ethylene polymerization with meso ansa metallocene-based catalysts)
IT 134876-98-5P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and **crystal** structure of meso ansa metallocene-based catalysts and branching formation in ethylene polymerization in presence of these catalysts)
IT 162429-20-1P **169103-22-4P** 192776-79-7P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of meso ansa metallocene-based catalysts and branching formation in ethylene **polymerization** in presence of these catalysts)
IT 917-54-4, Methyllithium 10026-11-6, Zirconium tetrachloride
13499-05-3, Hafnium tetrachloride 217494-94-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant in catalyst preparation; preparation of meso ansa metallocene-based
catalysts and branching formation in ethylene polymerization in presence of these catalysts)
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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IT **169103-22-4P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of meso ansa metallocene-based catalysts and branching formation in ethylene **polymerization** in presence of these catalysts)

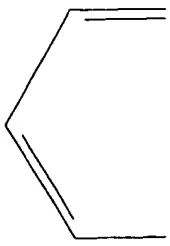
RN 169103-22-4 HCAPLUS

CN Zirconium(1+), [rel-(7aR,7'aS)-1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]methyl-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

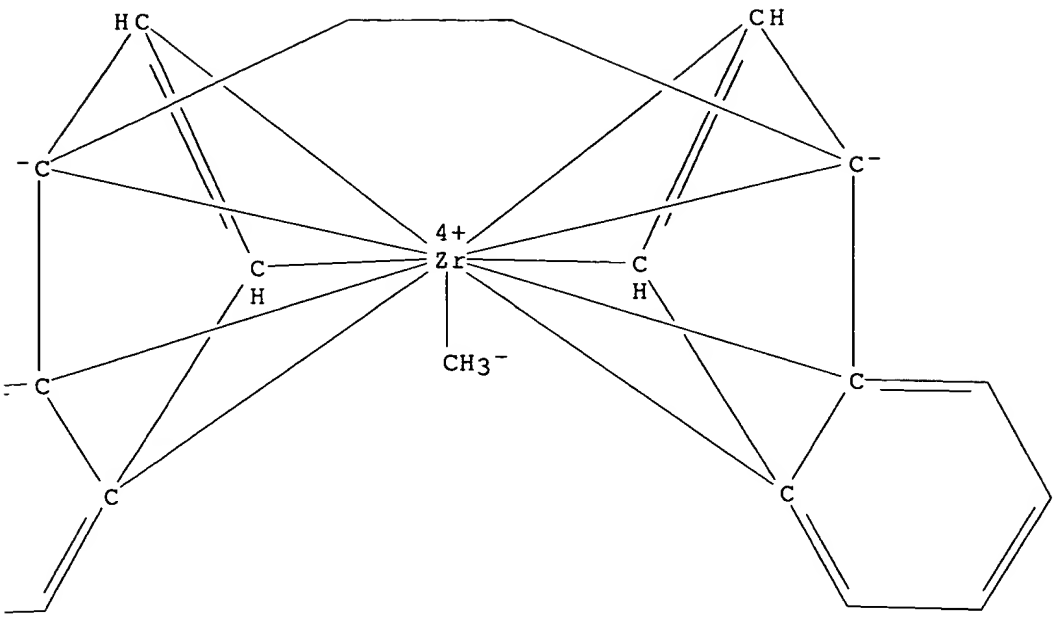
CM 1

CRN 169103-21-3
CMF C21 H19 Zr
CCI CCS

PAGE 1-A

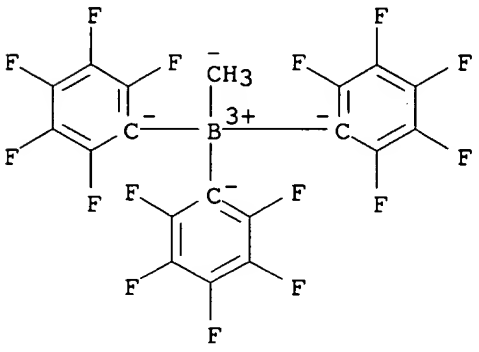


PAGE 1-B



CM 2

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



L34 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:834152 HCAPLUS
DN 138:187868
ED Entered STN: 03 Nov 2002
TI The reaction of (butadiene)zirconocene with imines
AU Holtke, Carsten; Erker, Gerhard; Kehr, Gerald; Frohlich, Roland; Kataeva, Olga
CS Organisch-Chemisches Institut der Universitat Munster, Munster, 48149, Germany

SO European Journal of Inorganic Chemistry (2002), (11), 2789-2799
CODEN: EJICFO; ISSN: 1434-1948
PB Wiley-VCH Verlag GmbH & Co. KGaA
DT Journal
LA English
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 75
OS CASREACT 138:187868

AB (Butadiene)zirconocene (s-trans-/s-cis-1 equilibrium mixture) reacts with the imine MeN=CHPh (7a) to form the 1:1 carbon-coupling product [κN-RN-CHPh-CH2-η3-(CHCH:CH2)]ZrCp2 (8a, R = Me). The x-ray **crystal** structure anal. of 8a revealed a metallacyclic structure featuring a distorted π-allyl moiety and a planar-tricoordinate nitrogen atom. Only one of the two possible diastereoisomers is found in the **crystal** (cis-8a) as well as in solution Treatment of 1 with the more bulky aldimine PhCH2N=CHPh (7b) selectively gave the corresponding 1:1 addition product trans-8b (R = PhCH2). Ketimines PhCH2N=C(CH2)4 (7c), HN=CPh2 (7d), or Δ1-2-methylpyrroline (7e) also reacted selectively with (butadiene)zirconocene to yield the analogous metallacyclic C-C coupling products [κN-RN-CR1R2-CH2-(η3-CHCH:CH2)]ZrCp2 (8c, R = PhCH2, R1-R2 = (CH2)4; 8d, R = H, R1 = R2 = Ph; 8e, R-R1 = (CH2)3, R2 = Me). Treatment of 8e with B(C6F5)3 proceeded cleanly by abstraction of a hydride anion from the carbon atom α to the nitrogen atom to form the intramolecularly coordinated imine product [Cp2Zr[4-[2-methyl-(κN-3,4-dihydro-2H-pyrrol-2-yl)]-(1,2,3-η)-2-butenyl]] 10 {isolated as [HB(C6F5)3-] salt 10a}. Similarly, Ph3C+ abstrs. a hydride ion from 8e to yield 10 {isolated as [B(C6H5)4-] salt 10b}. Proton addition from HNR3+ reagents takes place selectively at the Zr-amido nitrogen atom of the complexes 8a or 8d to yield the substituted (π-allyl) zirconocene cation complexes [Cp2Zr[(1,2,3-η)-CH2CH:CH-CH2CR1R2NHR3-κN]] (11, R1 = H, R2 = Ph, R3 = Me; 12, R1 = R2 = Ph, R3 = H), resp., isolated as BPh4- (a) or B(C6F5)3- (b) salts. The cationic complexes 10, 11, and 12 polymerize ethene at room temperature/2 bar of ethene with moderate catalytic activities.

ST zirconocene butadiene addn imine coupling amido allyl complex prepn; aldimine ketimine pyrroline oxazole addn zirconocene butadiene; hydride abstraction amido allyl zirconocene pyrrolinylallyl cation prepn; protonation amido allyl zirconocene aminoallyl cation complex prepn; ethylene polymn zirconocene aminoallyl cation complex prepn; **crystal** structure zirconocene amido allyl complex; mol structure zirconocene amido allyl complex

IT Coupling reaction
(addition of imines to zirconocene-butadiene complex to give amido-π-allyl metallacyclic zirconocene derivs.)

IT Imines
RL: RCT (Reactant); RACT (Reactant or reagent)
(addition of imines to zirconocene-butadiene complex to give amido-π-allyl metallacyclic zirconocene derivs.)

IT Functional groups
(allyl group, zirconocene complexes; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

IT Amines, preparation
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(amido complexes, protonation, hydride abstraction, ethylene polymerization; preparation of zirconocene amido-π-allyl metallacyclic complexes and

their protonation and hydride abstraction reactions and catalytic properties)

IT Polymerization catalysts
(coordination; preparation of zirconocene amido-π-allyl metallacyclic complexes and their catalytic activity in ethylene polymerization)

IT **Crystal** structure
Molecular structure
(of zirconocene amido-π-allyl complexes prepared by imines addition and coupling with zirconocene-butadiene complex)

IT Abstraction reaction
(preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

IT Metallacycles
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(protonation, hydride abstraction, ethylene polymerization; addition of imines to zirconocene-butadiene complex to give amido-π-allyl metallacyclic zirconocene derivs.)

IT 100-99-2, Triisobutylaluminum, uses
RL: CAT (Catalyst use); USES (Uses)
(co-catalyst; preparation of zirconocene amido-π-allyl metallacyclic complexes and their catalytic activity in ethylene polymerization)

IT 622-29-7 780-25-6 872-32-2 1013-88-3, Benzophenone imine 1120-64-5 15814-19-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(complexation, coupling; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

IT 499212-26-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(**crystal** structure, protonation; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

IT 499212-28-1P 499212-30-5P 499212-37-2P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(**crystal** structure; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

IT 499212-40-7P **499212-49-6P 499212-54-3P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(ethylene **polymerization**; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

IT 1109-15-5, Tris(pentafluorophenyl)borane 117802-41-2, Trityl tetraphenylborate
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydride abstraction; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

IT 499212-35-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydride abstraction; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction

reactions and catalytic properties)
IT 75374-50-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(imine addition, coupling; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)
IT 74-85-1, Ethene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(polymerization; preparation of zirconocene amido-π-allyl metallacyclic complexes and their catalytic activity in ethylene polymerization)
IT 9002-88-4P, Polyethylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of zirconocene amido-π-allyl metallacyclic complexes and their catalytic activity in ethylene polymerization)
IT 499212-43-0P 499212-47-4P 499212-52-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)
IT 64167-39-1 118612-00-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(protonation; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)
IT 499212-32-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(protonation; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)
RE.CNT 109 THERE ARE 109 CITED REFERENCES AVAILABLE FOR THIS RECORD
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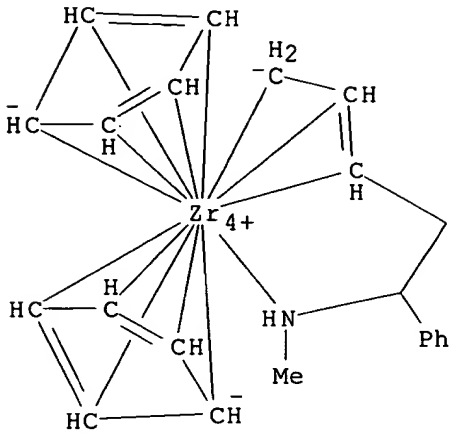
IT **499212-49-6P 499212-54-3P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(ethylene **polymerization**; preparation of zirconocene amido-π-allyl metallacyclic complexes and their protonation and hydride abstraction reactions and catalytic properties)

RN 499212-49-6 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)[(1,2,3-η)-(2E)-5-(methylamino-κN)-5-phenyl-2-pentenyl]-, stereoisomer, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

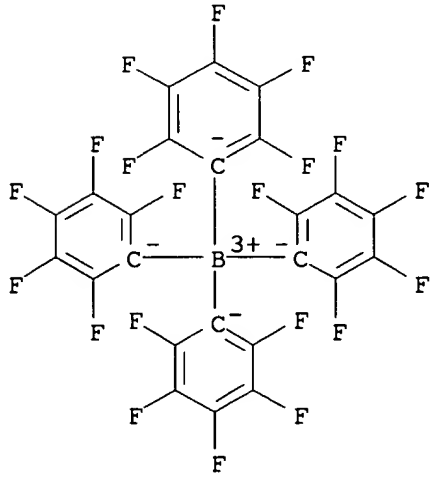
CM 1

CRN 524714-21-4
CMF C22 H26 N Zr
CCI CCS



CM 2

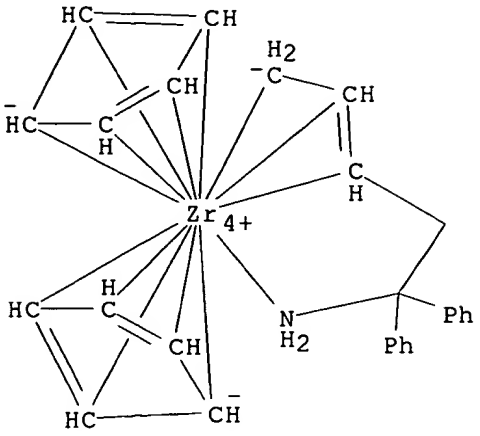
CRN 47855-94-7
CMF C24 B F20
CCI CCS



RN 499212-54-3 HCAPLUS
CN Zirconium(1+), [(1,2,3-η)-(2E)-5-(amino-κN)-5,5-diphenyl-2-pentenyl]bis(η5-2,4-cyclopentadien-1-yl)-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

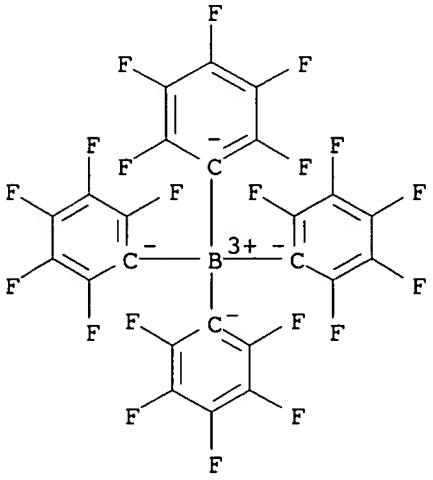
CM 1

CRN 499212-51-0
CMF C27 H28 N Zr
CCI CCS



CM 2

CRN 47855-94-7
CMF C24 B F20
CCI CCS



L34 ANSWER 5 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:688186 HCAPLUS
DN 137:239720
ED Entered STN: 11 Sep 2002
TI One-component photocurable resist composition for electronic parts
IN Hiwasa, Nobu
PA Otex K. K., Japan
SO Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC ICM C08G059-72

ICS C09K003-00
CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 37, 76
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 2002256063	A2	20020911	JP 2001-55168	20010228
PRAI JP 2001-55168		20010228		

OS MARPAT 137:239720
AB The composition comprises (a) cation-polymerizable organic substances of methylol compds., ethylenically unsatd. compds., and/or heterocyclic compds. 0.1-95, (b) latent photopolymn. initiators of **crystalline** ion-association substances represented by [{C5(R1)n}2mMm]l+[{B(R2)4}-]l [M = Fe; C5 = cyclopentadienyl; R1 = electron-donating alkyl group bonded to C of C5; n = 5; m = l = 1; R2 = (halogenated) aryl or halogenated alkyl ligand coordinated to B atom; 4 of R2 have same identity] 0.01-10, and (c) sensitizers 0.1-10%. The composition may contain 0.5-90% inorg. fillers. The composition is used for patterning resists, solder resists, plating resists, hole-embedding inks and resists, and conductive inks.
ST photocurable resist cation polymerizable org substance; ion assocn substance latent photopolymn initiator resist; sensitizer latent photopolymn initiator one component resist; methylol cation polymerizable photoresist elec part; unsatd compd cation polymerizable photoresist elec part; heterocyclic compd cation polymerizable photoresist elec part
IT Ethers, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(cyclic; one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for electronic parts)
IT Inks
(elec. conductive; one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for electronic parts)
IT Electric conductors
(inks; one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for electronic parts)
IT Photoresists
Printed circuit boards
Solder resists
(one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for electronic parts)
IT Cyclosiloxanes
Epoxides
Epoxy resins, uses
Lactams
RL: TEM (Technical or engineered material use); USES (Uses)
(one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for electronic parts)
IT Polymerization catalysts
(photopolymn., latent; one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for electronic parts)
IT 1344-28-1, Alumina, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(Admafine AO 802, filler; one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for

electronic parts)
IT 141-78-6, Acetidin, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(acetidin; one-component photoresist composition containing cation-polymerizable
substances, latent initiators, and sensitizers for electronic parts)
IT 471-34-1, Calcium carbonate, uses 7631-86-9, SO-E2, uses
RL: TEM (Technical or engineered material use); USES (Uses)
(filler; one-component photoresist composition containing cation-polymerizable
substances, latent initiators, and sensitizers for electronic parts)
IT **220517-46-4**
RL: **CAT (Catalyst use)**; USES (Uses)
(one-component photoresist composition containing cation-**polymerizable**
substances, latent initiators, and sensitizers for electronic parts)
IT 56-81-5D, Glycerin, polyglycidyl ether 95-96-5, Lactide 96-08-2, Limonene dioxide 109-99-9, Tetrahydrofuran, uses 110-88-3, Trioxane, uses 122-60-1, Phenyl glycidyl ether 123-91-1, Dioxane, uses 151-56-4, Aziridine, uses 286-20-4, Cyclohexene oxide 503-30-0, Oxetane 592-90-5, Oxepane 646-06-0, Dioxolane 930-22-3 1072-43-1, Propylene sulfide 2238-07-5, Diglycidyl ether 2386-90-5, Bis(2,3-epoxycyclopentyl) ether 2426-08-6, Butyl glycidyl ether 2451-62-9, Triglycidyl isocyanurate 4206-61-5, Diethylene glycol diglycidyl ether 5493-45-8 6303-21-5D, Phosphinic acid, esters 10580-65-1, Nonyl glycidyl ether 13410-52-1 13561-08-5, 2,6-Diglycidyl phenylglycidyl ether 13598-36-2D, Phosphonic acid, esters 16096-31-4, 1,6-Hexanediol diglycidyl ether 17557-23-2, Neopentyl glycol diglycidyl ether 18425-64-4, Trimethylolpropane diglycidyl ether 26142-30-3, Polypropylene glycol diglycidyl ether 26283-70-5, Epikote YL 6663 26403-72-5, Polyethylene glycol diglycidyl ether 26447-14-3, Cresyl glycidyl ether 28768-32-3 30424-08-9 30969-75-6, Oxazoline 58421-55-9, Epiclon 830S 65992-66-7, 1,3-Bis(N,N-diglycidylaminomethyl)cyclohexane 92308-50-4, RE 305 172416-00-1, Aron Oxetane OXT 121
RL: TEM (Technical or engineered material use); USES (Uses)
(one-component photoresist composition containing cation-polymerizable
substances, latent initiators, and sensitizers for electronic parts)
IT 56-55-3, 1,2-Benzoanthracene 81-64-1, Quinizarin 82-34-8, 1-Nitroanthraquinone 84-11-7, 9,10-Phenanthrenedione 84-51-5, 2-Ethylanthraquinone 84-54-8, 2-Methylanthraquinone 84-65-1, Anthraquinone 85-52-9, o-Benzoylbenzoic acid 90-44-8, Anthrone 90-47-1, Xanthone 90-96-0, 4,4'-Dimethoxybenzophenone 92-91-1 93-04-9, 2-Methoxynaphthalene 98-86-2, Acetophenone, uses 98-86-2D, Acetophenone, dimethoxy deriv 100-06-1 117-80-6, 2,3-Dichloro-1,4-naphthoquinone 119-61-9, Benzophenone, uses 120-12-7, Anthracene, uses 131-09-9, 2-Chloroanthraquinone 131-58-8, 2-Methylbenzophenone 134-81-6, Benzil 134-84-9, 4-Methylbenzophenone 256-81-5, 5H-Dibenzo[a,d]cycloheptene 492-22-8, Thioxanthone 527-61-7, 2,6-Dimethyl-1,4-benzoquinone 574-09-4, 2-Ethoxy-2-phenylacetophenone 605-94-7, 2,3-Dimethoxy-5-methyl-1,4-benzoquinone 606-28-0, Methyl o-benzoylbenzoate 611-94-9, 4-Methoxybenzophenone 611-99-4, 4,4'-Dihydroxybenzophenone 615-93-0, 2,5-Dichloro-p-benzoquinone 643-65-2, 3-Methylbenzophenone 829-20-9 1137-42-4, 4-Hydroxybenzophenone 1201-38-3 1210-12-4, 9-Cyanoanthracene 1210-35-1, Dibenzosuberone 1217-45-4, 9,10-Dicyanoanthracene 1676-63-7 2040-04-2 2128-93-0, 4-Phenylbenzophenone 2498-66-0, 1,2-Benzanthraquinone 2571-39-3, 3,4-Dimethylbenzophenone 2880-58-2 3524-62-7, Benzoin methyl ether 4044-60-4, 2,5-Dimethylbenzophenone

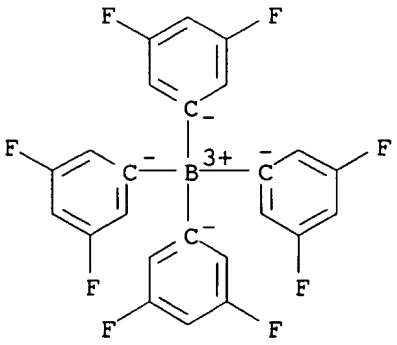
6175-45-7, Diethoxyacetophenone 6652-28-4, Benzoin isopropyl ether 10354-00-4, Dibenzosuberenol 10373-78-1, Camphorquinone 13020-57-0, 3-Hydroxybenzophenone 15774-82-0, 2-Methylthioxanthone 17214-11-8 25620-59-1, Aminoanthraquinone 26708-04-3, 2-Ethyl-9,10-dimethoxyanthracene 27938-76-7, Hydroxyanthraquinone 30587-18-9, Anisoin 30637-95-7, Anthraquinonesulfonic acid 41295-28-7, 3,3'-Dimethyl-4-methoxybenzophenone 75081-21-9, Isopropylthioxanthone 76293-13-5, 2,4-Dimethylthioxanthone 79044-56-7 82799-44-8, 2,4-Diethylthioxanthone 83846-85-9, 4-Benzoyl-4'-methyl-diphenyl sulfide 182683-80-3 457652-97-0
RL: TEM (Technical or engineered material use); USES (Uses)
(sensitizer; one-component photoresist composition containing cation-polymerizable substances, latent initiators, and sensitizers for electronic parts)

IT **220517-46-4**
RL: **CAT (Catalyst use)**; USES (Uses)
(one-component photoresist composition containing cation-**polymerizable** substances, latent initiators, and sensitizers for electronic parts)

RN 220517-46-4 HCAPLUS
CN Ferrocenium, decamethyl-, tetrakis(3,5-difluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

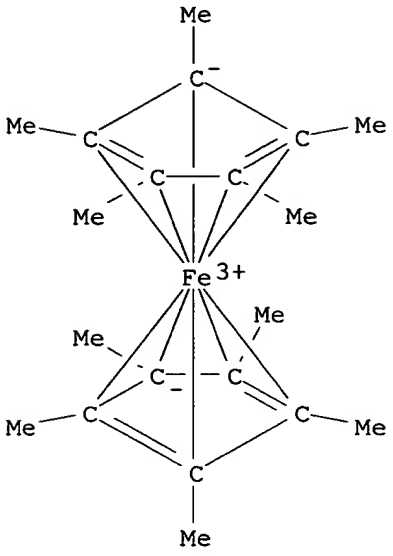
CM 1

CRN 153514-62-6
CMF C24 H12 B F8
CCI CCS



CM 2

CRN 54182-41-1
CMF C20 H30 Fe
CCI CCS



L34 ANSWER 6 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:357829 HCAPLUS
DN 137:93824
ED Entered STN: 14 May 2002
TI Reactivity of Zirconium Complexes Incorporating Asymmetrically Substituted ansa Ligands and Their Use as Catalysts in Olefin Polymerization. X-ray **Crystal** Structures of [Me2Si(η5-C5Me4)(η5-C5H3R)]ZrCl2 (R = Et, iPr)
AU Antinolo, Antonio; Lopez-Solera, Isabel; Otero, Antonio; Prashar, Sanjiv; Rodriguez, Ana M.; Villasenor, Elena
CS Departamento de Quimica Inorganica, Organica y Bioquimica, Universidad de Castilla-La Mancha, Facultad de Quimicas, Ciudad Real, 13071, Spain
SO Organometallics (2002), 21(12), 2460-2467
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 75
OS CASREACT 137:93824
AB The synthesis and use of the ansa-zirconocene complexes [Me2Si(η5-C5Me4)(η5-C5H3R)]ZrCl2 (R = H (5), Me (6), Et (7), iPr (8), tBu (9), SiMe3 (10)) as catalysts in the polymerization of ethylene and propylene has been studied. The alkyl complexes [Me2Si(η5-C5Me4)(η5-C5H3R)]ZrMe2 (R = H (11), Me (12), Et (13), iPr (14), tBu (15), SiMe3 (16)) have also been prepared The reaction of 11-16 with B(C6F5)3 gave the cationic species [{Me2Si(η5-C5Me4)(η5-C5H3R)}ZrMe]+ (R = H (17), Me (18), Et (19), iPr (20), tBu (21), SiMe3 (22)). In the absence of cocatalyst, 17-22 have been shown to act as catalysts in the polymerization of ethylene. The mol. structures of 7 and 8 have been determined by single-**crystal** x-ray diffraction studies.
ST asym silyl bridged ansa zirconocene complex prepn polymn catalyst; ansa zirconocene methyl asym silyl bridged prepn reaction fluorophenylborane; **crystal** mol structure asym silyl bridged ansa zirconocene complex

IT Aluminoxanes
RL: CAT (Catalyst use); USES (Uses)
(Me; reactivity of zirconium complexes incorporating asym. substituted ansa ligands and use as catalysts in olefin polymerization)
IT **Crystal** structure
Molecular structure
(of silyl bridged asym. substituted ansa zirconocene chloro complexes)
IT Polymerization catalysts
(reactivity of zirconium complexes incorporating asym. substituted ansa ligands and use as catalysts in olefin polymerization)
IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactivity of zirconium complexes incorporating asym. substituted ansa ligands and use as catalysts in olefin polymerization)
IT 324025-99-2
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(**crystal** structure, methylation, and polymerization of ethylene and propylene catalyzed by)
IT 139665-33-1 251292-39-4 324025-98-1
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(methylation and polymerization of ethylene and propylene catalyzed by)
IT 164598-03-2P 442689-81-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and lithiation of)
IT **442689-91-0P 442689-92-1P 442689-93-2P**
442689-94-3P 442689-95-4P 442689-96-5P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and **polymerization** of ethylene catalyzed by)
IT 442689-85-2P 442689-86-3P 442689-87-4P 442689-88-5P 442689-89-6P
442689-90-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with tris(pentafluorophenyl)borane)
IT 162369-26-8P 442689-82-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with zirconium tetrachloride)
IT 442689-83-0P
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, **crystal** structure, methylation, and polymerization of ethylene and propylene catalyzed by)
IT 442689-84-1P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, methylation, and polymerization of ethylene and propylene catalyzed
by)
IT 1109-15-5, Tris(pentafluorophenyl)borane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with asym. substituted silyl bridged ansa zirconocene Me complex)
IT 74-85-1, Ethylene, reactions 115-07-1, Propylene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(reactivity of zirconium complexes incorporating asym. substituted ansa ligands and use as catalysts in olefin polymerization)

IT 9002-88-4P, Polyethylene 9003-07-0P, Polypropylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(reactivity of zirconium complexes incorporating asym. substituted ansa ligands and use as catalysts in olefin polymerization)

IT 50356-03-1 211058-86-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction of chloroorganosilane with)

IT 125542-03-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(substitution reaction with bis(ethylcyclopentadienyl)magnesium)

RE.CNT 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD

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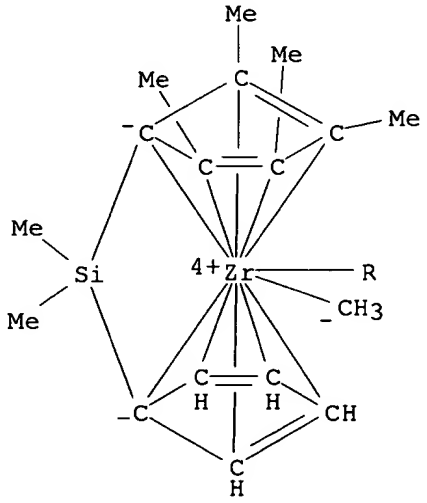
IT **442689-91-0P 442689-92-1P 442689-93-2P 442689-94-3P 442689-95-4P 442689-96-5P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and **polymerization** of ethylene catalyzed by)

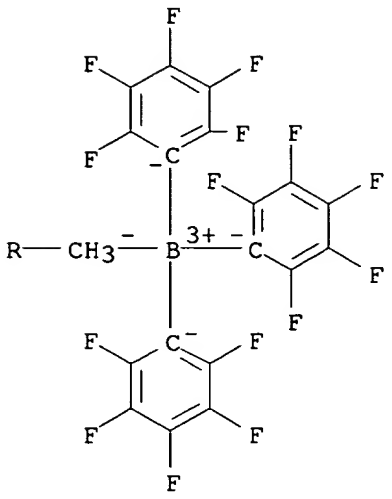
RN 442689-91-0 HCAPLUS

CN Zirconium, [η10-2,4-cyclopentadien-1-ylidene(dimethylsilylene)(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)]-μ-methylmethyl[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

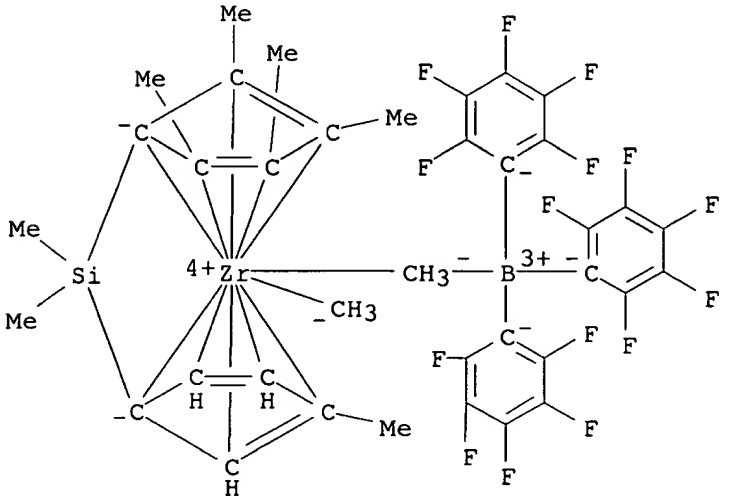
PAGE 1-A



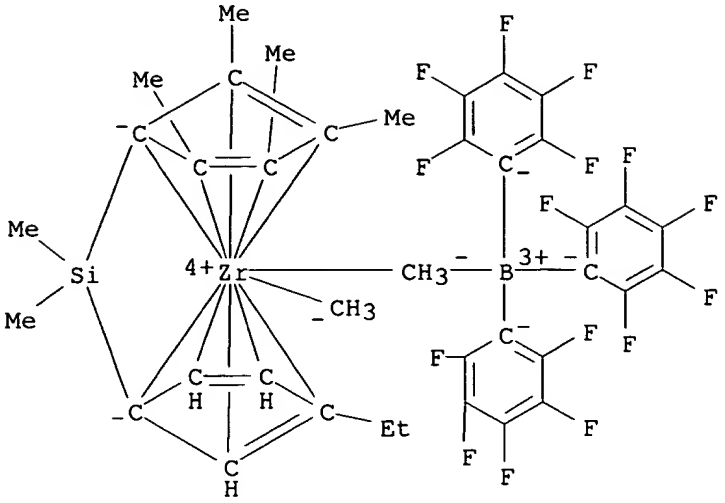
PAGE 2-A



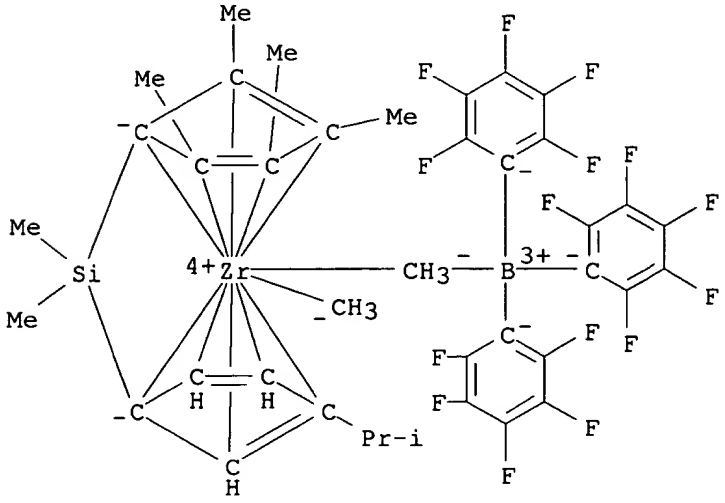
RN 442689-92-1 HCAPLUS
CN Zirconium, μ-methylmethyl[η10-(3-methyl-2,4-cyclopentadien-1-ylidene)(dimethylsilylene)(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)][tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)



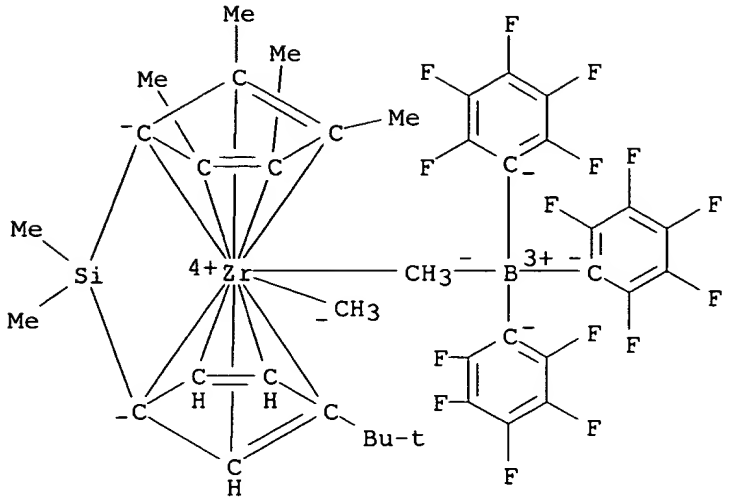
RN 442689-93-2 HCAPLUS
CN Zirconium, [η10-(3-ethyl-2,4-cyclopentadien-1-ylidene)(dimethylsilylene)(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)]-μ-methylmethyl[tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)



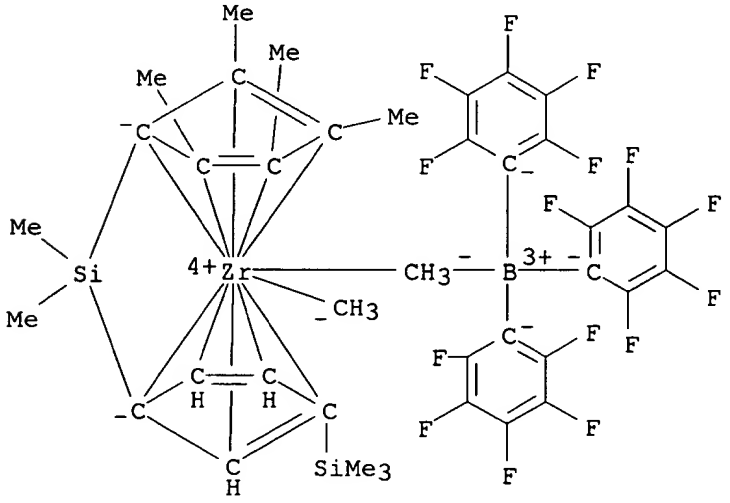
RN 442689-94-3 HCAPLUS
CN Zirconium, μ-methylmethyl[η10-[3-(1-methylethyl)-2,4-cyclopentadien-1-ylidene](dimethylsilylene)(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)][tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)



RN 442689-95-4 HCAPLUS
CN Zirconium, [η10-[3-(1,1-dimethylethyl)-2,4-cyclopentadien-1-ylidene](dimethylsilylene)(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)]-μ-methylmethyl[tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)

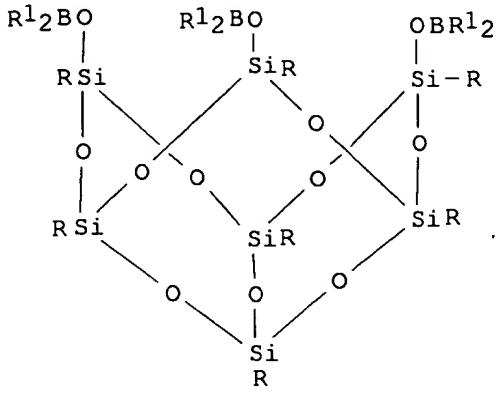


RN 442689-96-5 HCAPLUS
CN Zirconium, μ-methylmethyl[η10-(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)(dimethylsilylene)[3-(trimethylsilyl)-2,4-cyclopentadien-1-ylidene]][tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)



L34 ANSWER 7 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:215368 HCAPLUS
DN 136:386179
ED Entered STN: 22 Mar 2002
TI Organoborane-Modified Silica Supports for Olefin Polymerization: Soluble Models for Metallocene Catalyst Deactivation
AU Metcalfe, Robert A.; Kreller, David I.; Tian, Jun; Kim, Hoon; Taylor, Nicholas J.; Corrigan, John F.; Collins, Scott
CS Department of Chemistry, University of Waterloo, Waterloo, ON, N2L 3G1, Can.
SO Organometallics (2002), 21(8), 1719-1726

CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-6 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 75
OS CASREACT 136:386179
GI



I

AB Treatment of silsesquioxane with 3.3 equiv of the reactive organoboranes [(C6F5)2BX; X = H or Cl] provides the novel, trifunctional organoborane I (R = cyclopentyl, R1 = pentafluorophenyl), which was characterized by spectroscopic and single-**crystal** x-ray **crystallog**.

Compound I is an effective cocatalyst for ethylene polymerization in combination with Cp2ZrMe2 but only when these two compds. are combined in situ, in the presence of monomer, suggesting limited stability of the putative ion-pair derived from these compds. Reaction of I with Cp2ZrMe2 in toluene solution leads to formation of MeB(C6F5)2- and Cp2Zr-functionalized silsesquioxane at room temperature Monitoring of this reaction by NMR spectroscopy at low temps. indicates that the only ion-pair present is [Cp2ZrMe][Me2B(C6F5)2] (4), which results from reaction of Cp2ZrMe2 with the byproduct MeB(C6F5)2. Formation of 4 is reversible under these conditions, while production of silsesquioxane (from I and Cp2ZrMe2) is not; the latter process occurs at a rate that exceeds that observed for independent decomposition of 4 to form Me2B(C6F5) and Cp2Zr(C6F5)Me. These studies suggest that the active polymerization catalyst generated in situ from I and Cp2ZrMe2 is probably ion-pair 4.

ST organo borane modified silica support prepn olefin polymn cocatalyst; dimethyl zirconocene catalyst boryloxy silsesquioxane cocatalyzed ethylene polymn; **crystal** mol structure fluorophenylboryloxy silsesquioxane
IT **Crystal** structure
Molecular structure
(of organoborane-modified silsesquioxane)

IT Polymerization catalysts
(preparation of organoborane-modified silica supports for olefin polymerization and
soluble models for metallocene catalyst deactivation)
IT **426827-42-1P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(formation, NMR, and ethylene **polymerization** catalyzed with)
IT 426827-43-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 12636-72-5, Dimethylzirconocene
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(preparation of organoborane-modified silica supports for olefin polymerization and
soluble models for metallocene catalyst deactivation)
IT 74-85-1, Ethylene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of organoborane-modified silica supports for olefin polymerization and
soluble models for metallocene catalyst deactivation)
IT 426827-40-9P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, **crystal** structure, reaction with
dimethylzirconocene, and ethylene polymerization cocatalyzed with)
IT 135225-24-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with chlorobis(pentafluorophenyl)borane)
IT 2720-03-8, Chlorobis(pentafluorophenyl)borane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with endo trisilanol)
IT 56252-55-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with organoborane-modified silsesquioxane)
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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IT **426827-42-1P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(formation, NMR, and ethylene **polymerization** catalyzed with)

RN 426827-42-1 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, (T-4)-dimethylbis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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CRN 426827-41-0
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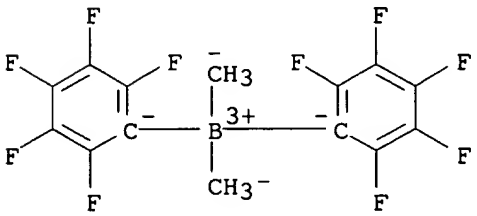
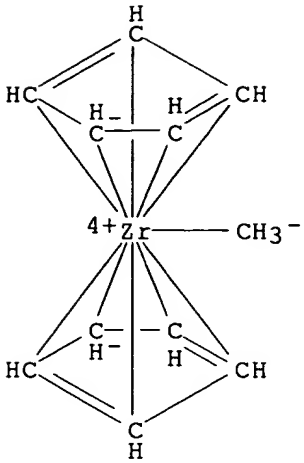
CCI CCS



CM 2

CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS



L34 ANSWER 8 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:6959 HCAPLUS
DN 136:216782
ED Entered STN: 04 Jan 2002
TI [H2N{B(C6F5)3}2]-: A New, Remarkably Stable Diborate Anion for Metallocene Polymerization Catalysts
AU Lancaster, Simon J.; Rodriguez, Antonio; Lara-Sanchez, Agustin; Hannant, Mark D.; Walker, Dennis A.; Hughes, David H.; Bochmann, Manfred
CS Wolfson Materials and Catalysis Centre School of Chemical Sciences, University of East Anglia, Norwich, NR4 7TJ, UK
SO Organometallics (2002), 21(3), 451-453
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 75
OS CASREACT 136:216782
AB The reaction between NaNH2 and B(C6F5)3 affords the amidodiborate anion [H2N{B(C6F5)3}2]-, the x-ray **crystal** structure of which shows multiple intramol. NH···F hydrogen bonding. Reaction with HCl affords [H(OEt2)2][H2N{B(C6F5)3}2], while treatment of zirconocene dimethyls with [CPh3][H2N{B(C6F5)3}2] gives highly active alkene polymerization catalysts.
ST amido diborate anion prepn metallocene polymn catalyst; fluorophenyl diborate amido anion prepn metallocene polymn catalyst
IT **Crystal** structure
Hydrogen bond
Molecular structure
(of pentafluorophenyl substituted amidodiborate anion)
IT Polymerization catalysts
(preparation of pentafluorophenyl substituted amidodiborate anion zirconocene complexes as)
IT 115-07-1, Propene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidodiborate/zirconocene complex catalyzed polymerization of)
IT **402828-29-9P 402828-30-2P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP

(Preparation); USES (Uses)
(preparation as alkene **polymerization** catalyst)
IT 402572-71-8P 402572-73-0P 402572-75-2P 402572-77-4P 402572-78-5P
402827-90-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 402572-70-7P
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, **crystal** structure, hydrogen bonding, reaction with trityl chloride and zirconocene complexes, and alkene polymerization cocatalysis with)
IT 75-24-1, Trimethylaluminum
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of zirconocene complexes with pentafluorophenyl substituted amidodiborate anion in presence of)
IT 131761-40-5 146814-57-5 204863-69-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with amidodiborate anion in presence of trimethylaluminum)
IT 76-83-5, Triphenylmethyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with pentafluorophenyl substituted amidodiborate anion)
IT 1109-15-5, Tris(pentafluorophenyl)borane
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with sodium amide)
RE.CNT 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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IT **402828-29-9P 402828-30-2P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as alkene **polymerization** catalyst)

RN 402828-29-9 HCAPLUS

CN Zirconium(1+), rel-bis[(1R,1'R)-(dimethylsilylene)bis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]-μ-methyldimethyldi-, μ-amidohexakis(pentafluorophenyl)diborate(1-) (9CI) (CA INDEX NAME)

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CRN 402572-69-4
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CCI CCS

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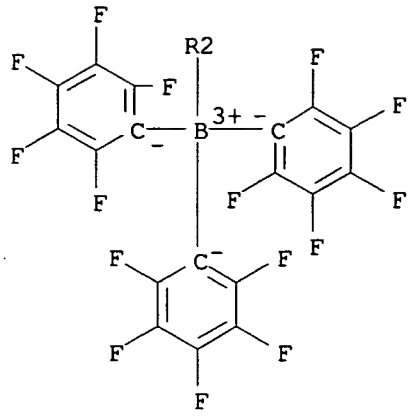

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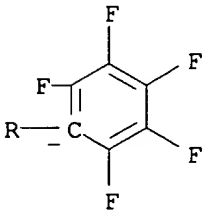

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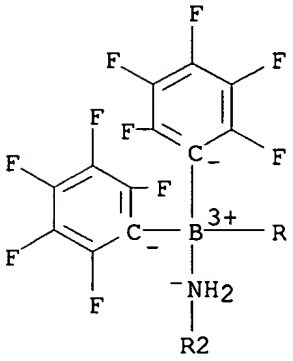

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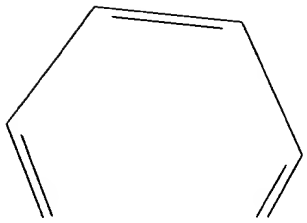
CRN 207003-99-4
CMF C43 H45 Si2 Zr2
CCI CCS

PAGE 1-A



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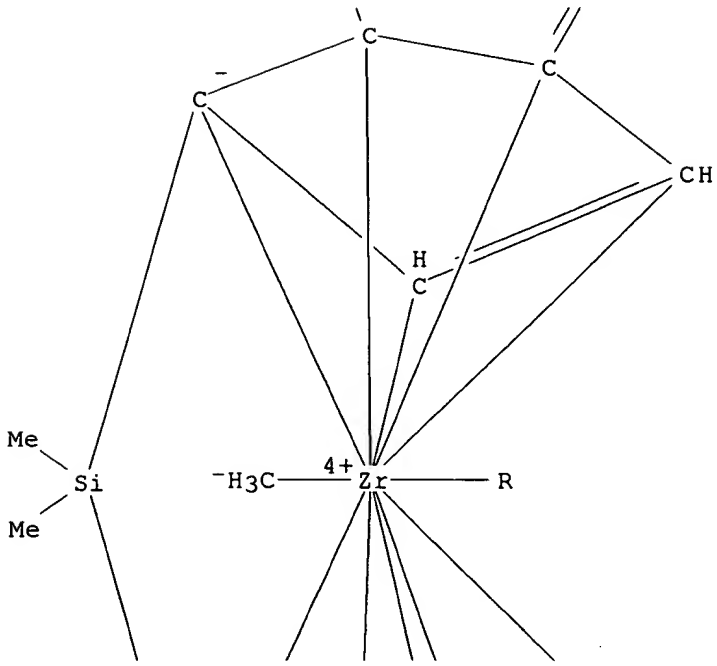

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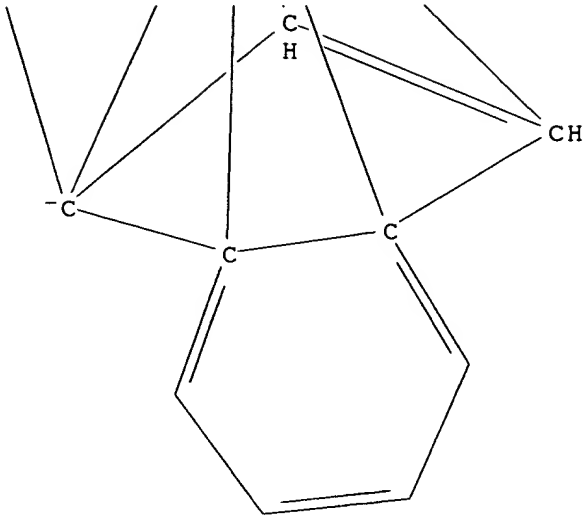

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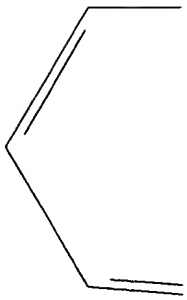

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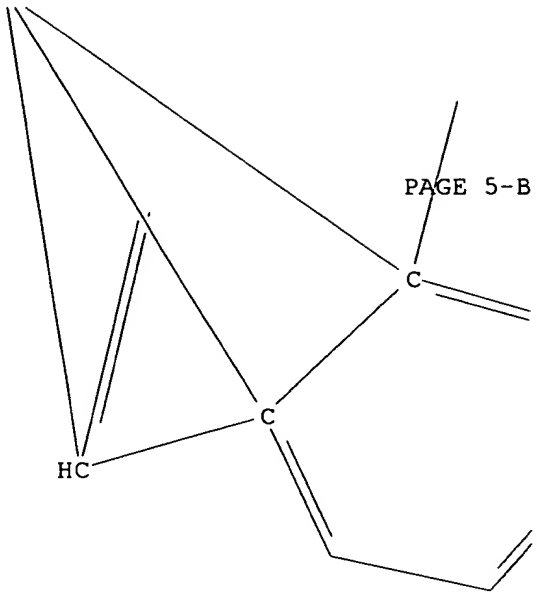


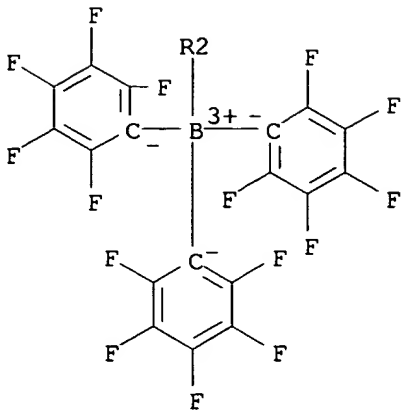
PAGE 5-C

RN 402828-30-2 HCAPLUS
CN Zirconium(1+), rel-[(1R,1'R)-(dimethylsilylene)bis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]][(1S,1'S)-(dimethylsilylene)bis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]-μ-methyldimethyldi-, μ-amidohexakis(pentafluorophenyl)diborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 402572-69-4
CMF C36 H2 B2 F30 N
CCI CCS

PAGE 1-A



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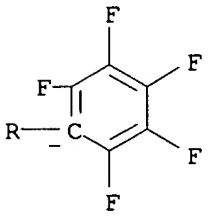

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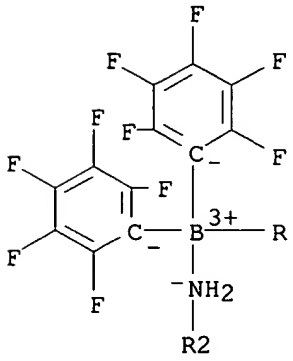

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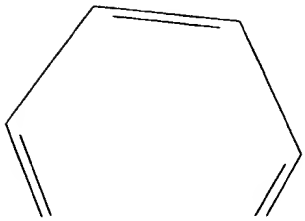
CRN 207004-02-2
CMF C43 H45 Si2 Zr2
CCI CCS

PAGE 1-A



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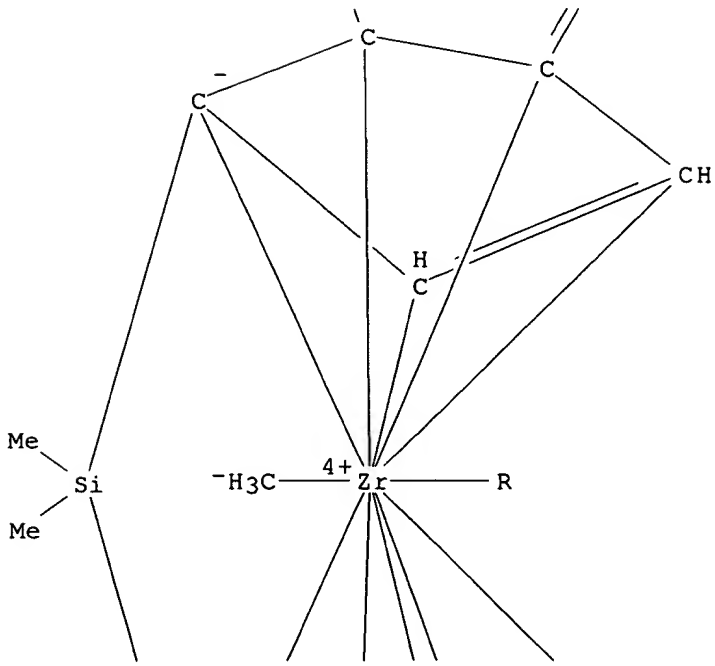

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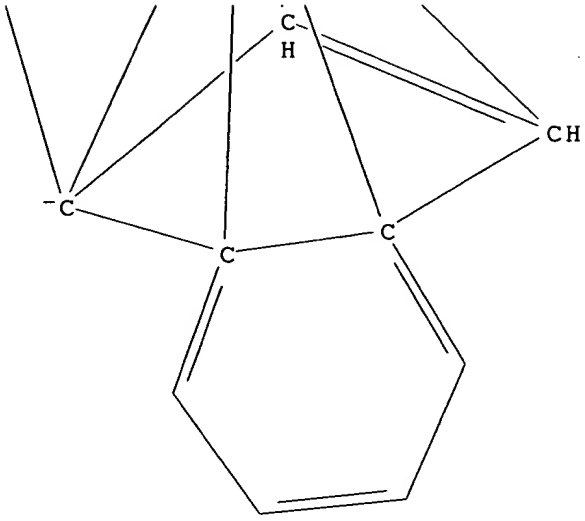

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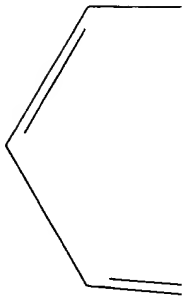

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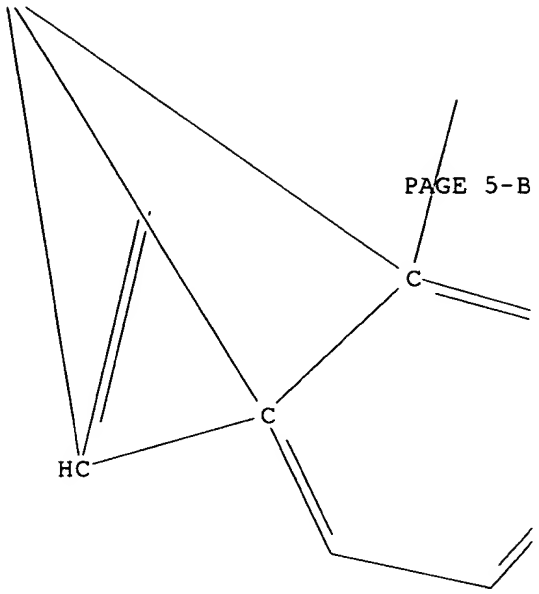

PAGE 5-C

L34 ANSWER 9 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:28166 HCAPLUS
DN 134:237878
ED Entered STN: 12 Jan 2001
TI "Double Activation" of Constrained Geometry and ansa-Metallocene Group 4 Metal Dialkyls: Synthesis, Structure, and Olefin Polymerization. Study of Mono- and Dicationic Aluminate Complexes
AU Chen, Eugene Y.-X.; Kruper, William J.; Roof, Gordon; Wilson, David R.
CS Corporate R&D, The Dow Chemical Company, Midland, MI, 48674, USA
SO Journal of the American Chemical Society (2001), 123(4), 745-746
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 75

AB The ability of Al(C6F5)3 for the formation of dicationic group 4 constrained geometry and ansa-metallocene bisaluminate complexes was investigated ("double activation"). One equiv of Al(C6F5)3 was reacted with complexes Me2Si(η5-Me4C5)(t-BuN)TiMe2 (CGC-TiMe2) and rac-Me2Si(η5-Ind)2-ZrMe2 (SBI-ZrMe2) to produce the corresponding stable and isolable cationic complexes CGC-TiMe(μ-Me)Al(C6F5)3 (I) and SBI-ZrMe(μ_Me)Al(C6F5)3 (II), which were fully characterized by spectroscopic and **crystallog**. methods. Addition of a 2nd equiv of Al(C6F5)3 to the toluene solution of I or II led to the formation of the corresponding dicationic bisaluminate complexes CGC-Ti[(μ-Me)Al(C6F5)3]2 (III) and SBI-Zr[(μ-Me)Al(C6F5)3]2 (IV). NMR and **crystallog**. data are consistent with geometry changes from C1-symmetry (I and II) to Cs-symmetry in III and C2-symmetry in IV. The influence of the catalyst double activation on polymerization characteristics was investigated using copolymn. of ethylene/1-octene under CGC-TiMe2 and SBI-ZrMe2 catalysis by adding 1 or multiple equivalent of B(C6F5)3 or Al(C6F5)3 to reaction mixture The dicationic complexes exhibited more efficient olefin polymerization activity than the corresponding mono-cationic catalysts.

ST olefin polymn catalyst metallocene aluminate complex; zirconocene aluminate complex prepn polymn catalyst; titanocene aluminate complex prepn polymn catalyst; ethylene octene polymn metallocene bisaluminate catalyst; metallocene aluminate complex prepn polymn catalyst; **crystal** structure titanocene zirconocene aluminate complex

IT Polymerization catalysts
(metallocene; preparation and activity of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT **Crystal** structure
Molecular structure
(of monocationic and dicationic constrained-geometry ansa-metallocene aluminate complexes)

IT 330455-80-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(**crystal** structure; preparation and properties of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT 219627-05-1P 330454-34-7P 330454-35-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(decomposition of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT 330454-32-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(mol. and **crystal** structure; preparation and activity of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT 258883-44-2P
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)
(mol. structure; preparation and properties of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT 193149-39-2P **326817-27-0P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and activity of dicationic metallocene bisaluminate complex catalysts for olefin **polymerization**)

IT 330454-33-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and activity of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT 1109-15-5, Tris(pentafluorophenyl)borane 135072-62-7 149197-69-3, rac-Dimethyl(dimethylsilylene)bis(1-indenyl)zirconium 168704-96-9, Tris(pentafluorophenyl)aluminum
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation and activity of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT 258883-18-0P
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); USES (Uses)
(preparation and properties of dicationic metallocene bisaluminate complex catalysts for olefin polymerization)

IT 26221-73-8P, Ethylene-1-octene copolymer
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation of polyolefins in presence of dicationic metallocene bisaluminate complex catalysts)

RE.CNT 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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IT **326817-27-0P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and activity of dicationic metallocene bisaluminate complex catalysts for olefin **polymerization**)

RN 326817-27-0 HCAPLUS

CN Zirconium, [rel-(1R,1'R)-(dimethylsilylene)bis[(1,2,3,3a,7a-η)-1H-

inden-1-ylidene]]-μ-methylmethyl[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

applicants

L34 ANSWER 10 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:553528 HCAPLUS
DN 133:164482
ED Entered STN: 11 Aug 2000
TI Novel **crystalline** ion-association substance, process for producing the same, and polymerization initiator
IN Hiwasa, Shin
PA Autex, Inc., Japan
SO PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC ICM C07C017-02
ICS C07C019-00; C08F004-603; C08F004-70; C08G085-00; C07F005-02; C07F015-02; C08G059-68
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 42
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000046171	A1	20000810	WO 2000-JP518	20000131
	W: CA, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	JP 2000226396	A2	20000815	JP 1999-24294	19990201
	EP 1153905	A1	20011114	EP 2000-902020	20000131
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
PRAI	JP 1999-24294	A	19990201		
	WO 2000-JP518	W	20000131		

OS MARPAT 133:164482
AB The title substance, i.e., a metallocene borate, initiates photopolymn. and thermal polymerization Thus, ferrocenium tetrakis(3,5-difluorophenyl) borate
was prepared and used as a catalyst for the polymerization of 1,3,5,7-tetramethylcyclotetracyclosiloxane to form a film.
ST cyclosiloxane polymn catalyst ferrocenium fluorophenyl borate; photopolymn catalyst metallocene borate; thermal polymn catalyst metallocene borate
IT Polymerization catalysts
(cationic; metallocene-borate **crystalline** ion-association substances for polymerization catalysts)
IT Phenolic resins, preparation
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(epoxy, novolak; metallocene-borate **crystalline** ion-association substances for polymerization catalysts)
IT Epoxy resins, preparation
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(hydrogenated; metallocene-borate **crystalline** ion-association substances for polymerization catalysts)
IT Functional groups
(hydroxymethyl group; metallocene-borate **crystalline** ion-association

substances for polymerization catalysts)
IT Coating materials
Electron donors
(metallocene-borate **crystalline** ion-association substances for polymerization
catalysts)
IT Coordination compounds
RL: CAT (Catalyst use); IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(metallocene-borate **crystalline** ion-association substances for polymerization
catalysts)
IT Polysiloxanes, preparation
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(metallocene-borate **crystalline** ion-association substances for polymerization
catalysts)
IT Borates
Cyclosiloxanes
Heterocyclic compounds
Metallocenes
Polyamides, reactions
Transition metal compounds
Unsaturated compounds
RL: RCT (Reactant); RACT (Reactant or reagent)
(metallocene-borate **crystalline** ion-association substances for polymerization
catalysts)
IT Epoxy resins, preparation
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(phenolic, novolak; metallocene-borate **crystalline** ion-association substances for polymerization catalysts)
IT Polymerization catalysts
(photopolymn.; metallocene-borate **crystalline** ion-association substances for polymerization catalysts)
IT Acetals
RL: RCT (Reactant); RACT (Reactant or reagent)
(polyacetals, nonpolymeric; metallocene-borate **crystalline** ion-association substances for polymerization catalysts)
IT Polymerization catalysts
(thermal; metallocene-borate **crystalline** ion-association substances for polymerization catalysts)
IT 119-61-9, Benzophenone, uses 1210-35-1
RL: CAT (Catalyst use); USES (Uses)
(metallocene-borate **crystalline** ion-association substances for polymerization
catalysts)
IT **143607-33-4P 156301-37-0P 288101-82-6P**
288101-83-7P 288101-84-8P 288101-85-9P
288101-86-0P 288101-88-2P 288101-89-3P
288101-90-6P 288101-91-7P 288101-92-8P
288101-93-9P
RL: **CAT (Catalyst use)**; IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(metallocene-borate **crystalline** ion-association substances for **polymerization** catalysts)

IT 108-95-2DP, Phenol, novolak epoxy resins, preparation 1333-16-0DP, Bisphenol F, epoxy resins 9004-73-3P, Poly(1,3,5,7-tetramethylcyclotetrasiloxane, SRU 9016-00-6P, Poly(octamethylcyclotetrasiloxane), SRU 25037-57-4P, Poly(octamethylcyclotetrasiloxane) 26710-23-6P 27576-78-9P, Poly(1,3,5,7-tetramethylcyclotetrasiloxane) 28323-47-9P, Poly(hexaethylcyclotrisiloxane), SRU 31305-85-8P, Poly(1,3-bis(glycidoxypropyl)tetramethyldisiloxane) 32625-53-9P, Decamethylcyclopentasiloxane homopolymer 65581-98-8P, Epiclon 830 88483-06-1P, Poly(hexaethylcyclotrisiloxane) 110294-68-3P 111319-45-0P 117932-09-9P, Poly(dodecamethylcyclohexasiloxane) 147881-71-8P, Epiclon N 730A 183867-42-7P, Poly[oxy(phenylsilylene)] 183867-43-8P 220175-12-2P, Epikote RXE 21 288101-94-0P
RL: IMF (Industrial manufacture); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)
(metallocene-borate **crystalline** ion-association substances for polymerization catalysts)

IT 102-54-5, Ferrocene 109-63-7, Boron trifluoride etherate 461-96-1, 1-Bromo-3,5-difluorobenzene 1291-47-0, Dimethylferrocene 2797-28-6 12152-94-2 12156-05-7 22533-15-9 31904-29-7, Butylferrocene 53954-86-2, tert-Amyl-ferrocene 66016-55-5, 1,2,4,1',2',4'-Hexamethylferrocene 79060-88-1 119861-51-7, Sodium tetrakis(3,5-difluorophenyl)borate
RL: RCT (Reactant); RACT (Reactant or reagent)
(metallocene-borate **crystalline** ion-association substances for polymerization catalysts)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Klimova, E; J Organomet Chem 1998, V559(1-2), P43 HCAPLUS
(2) Pcd Polymere Gesellschaft m B H; EP 673946 A2 HCAPLUS
(3) Pcd Polymere Gesellschaft m B H; JP 841088 A
(4) Pcd Polymere Gesellschaft m B H; US 5521265 A 1996 HCAPLUS
(5) Studiengesellschaft Kohle Mbh; JP 11152295 A HCAPLUS
(6) Studiengesellschaft Kohle Mbh; EP 897926 A1 HCAPLUS
(7) Studiengesellschaft Kohle Mbh; US 5959132 A 1999 HCAPLUS

IT **143607-33-4P 156301-37-0P 288101-82-6P 288101-83-7P 288101-84-8P 288101-85-9P 288101-86-0P 288101-88-2P 288101-89-3P 288101-90-6P 288101-91-7P 288101-92-8P 288101-93-9P**
RL: **CAT (Catalyst use)**; IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(metallocene-borate **crystalline** ion-association substances for **polymerization** catalysts)

RN 143607-33-4 HCAPLUS

CN Ferrocenium, 1,1'-dimethyl-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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CRN 47855-94-7
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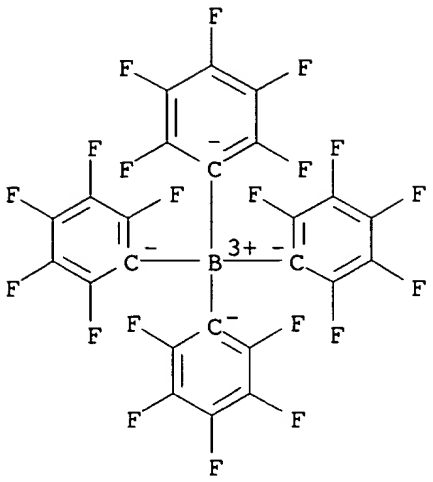
CCI CCS



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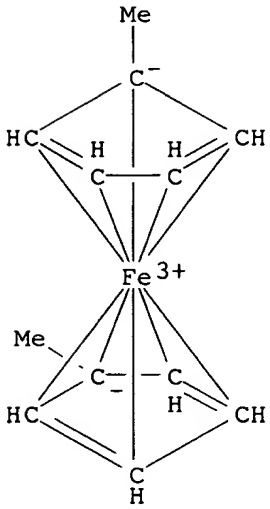
CCI CCS



RN 156301-37-0 HCAPLUS
CN Ferrocenium, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (9CI) (CA INDEX NAME)

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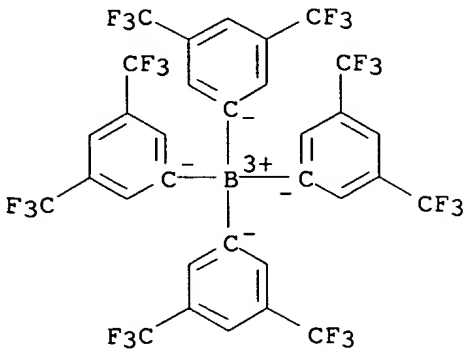
CCI CCS



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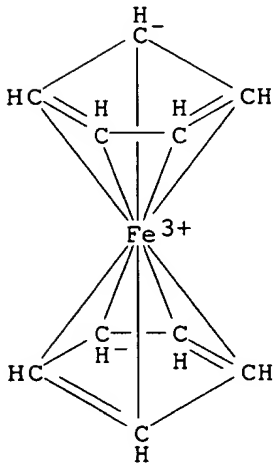

RN 288101-82-6 HCAPLUS
CN Ferrocenium, tetrakis(3,5-difluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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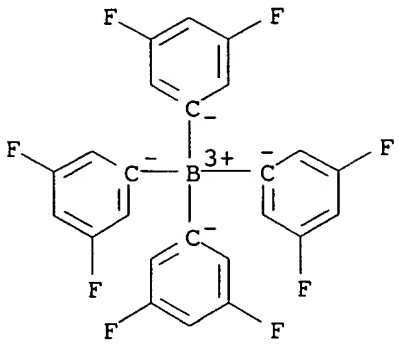

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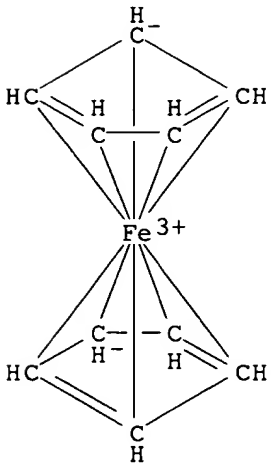

RN 288101-83-7 HCAPLUS
CN Ferrocenium, 1,1'-dimethyl-, tetrakis(3,5-difluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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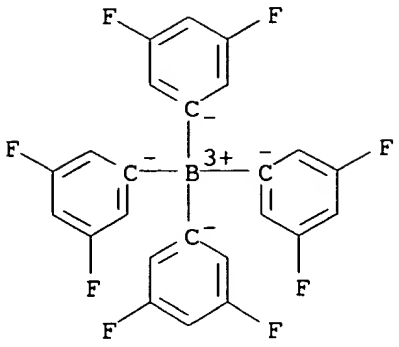
CCI CCS



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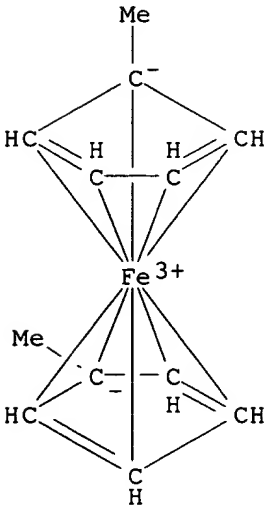
CCI CCS



RN 288101-84-8 HCAPLUS
CN Ferrocenium, 1,1',2,2',4,4'-hexamethyl-, tetrakis(3,5-difluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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CRN 153514-62-6
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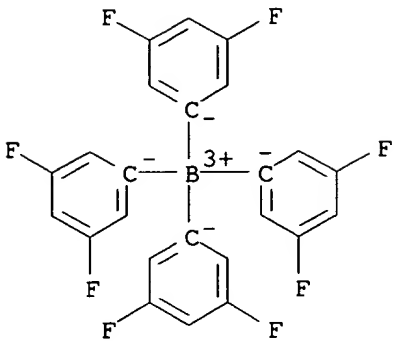
CCI CCS



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CRN 66016-55-5
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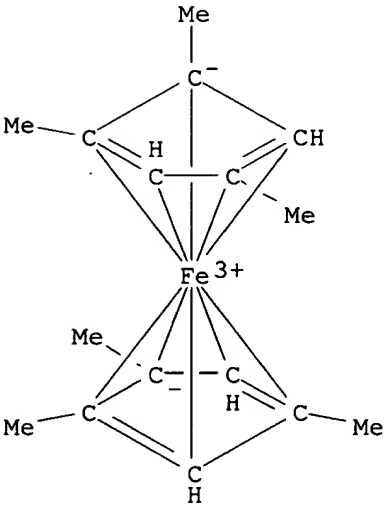
CCI CCS



RN 288101-85-9 HCAPLUS
CN Ferrocenium, butyl-, tetrakis(3,5-difluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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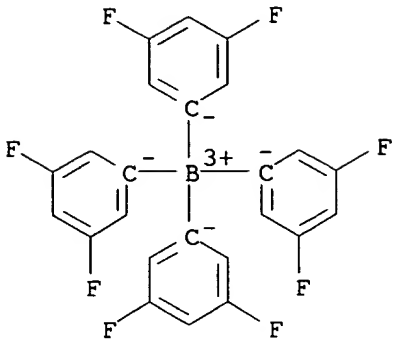
CMF C24 H12 B F8
CCI CCS



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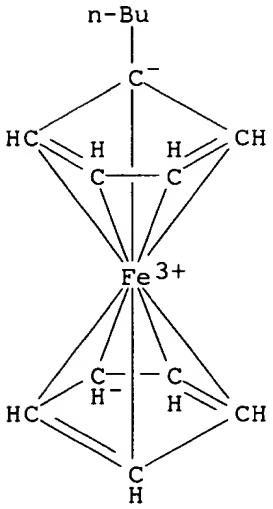

RN 288101-86-0 HCAPLUS
CN Ferrocenium, (1,1-dimethylpropyl)-, tetrakis(3,5-difluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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CRN 153514-62-6
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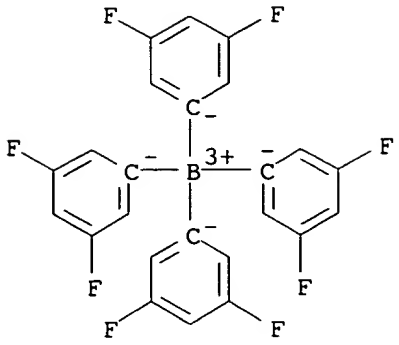
CCI CCS



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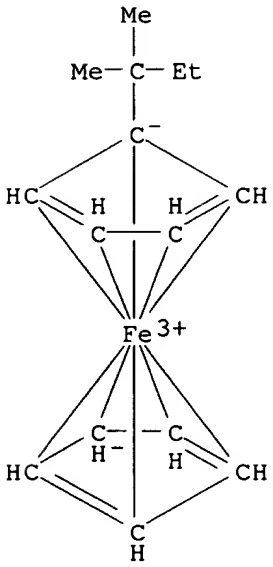

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CN Ferrocenium, borono-, tetrakis(3,5-difluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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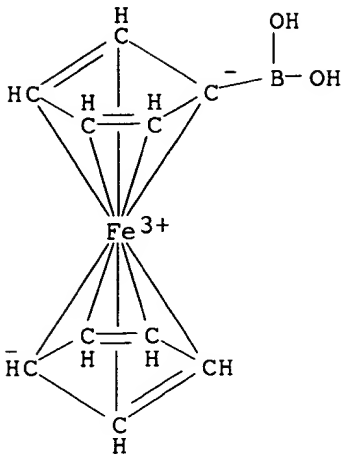
CCI CCS



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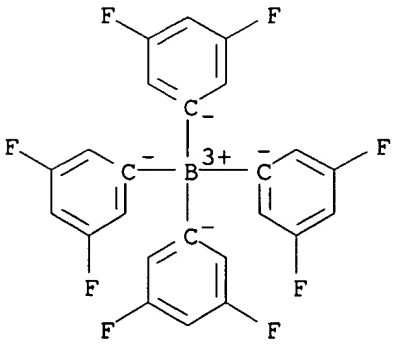

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CN Ferrocenium, 1,1'-dimethyl-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borat e(1-) (9CI) (CA INDEX NAME)

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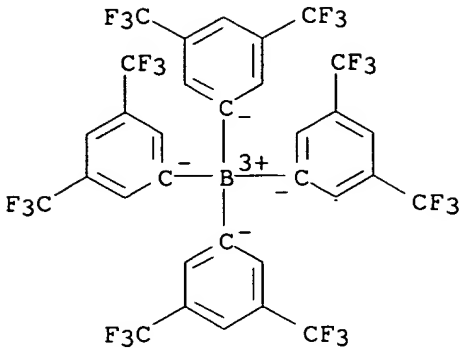

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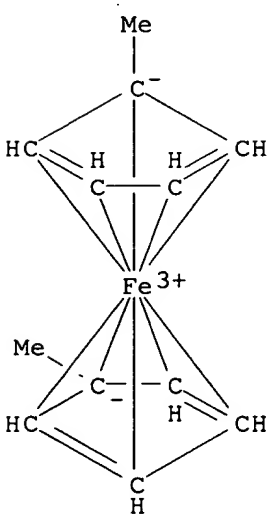

RN 288101-90-6 HCAPLUS
CN Ferrocenium, 1,1',2,2',4,4'-hexamethyl-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (9CI) (CA INDEX NAME)

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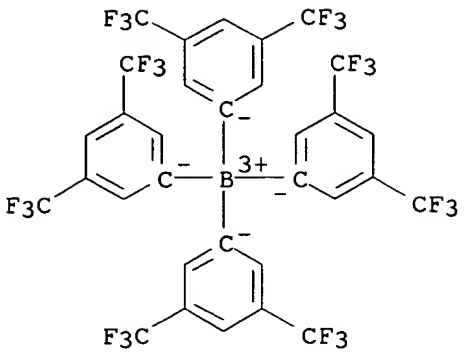
CRN 79230-20-9
CMF C32 H12 B F24
CCI CCS



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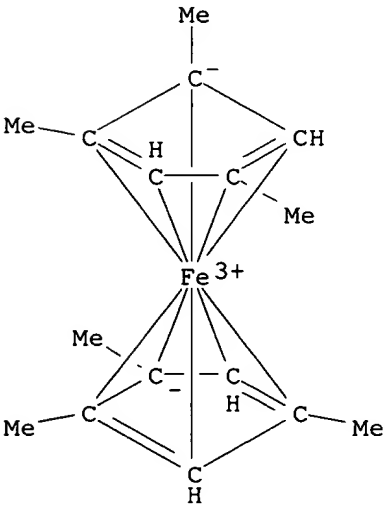

RN 288101-91-7 HCAPLUS
CN Ferrocenium, 1,1',2,2',4,4'-hexamethyl-, tetrakis(pentafluorophenyl)borate (1-) (9CI) (CA INDEX NAME)

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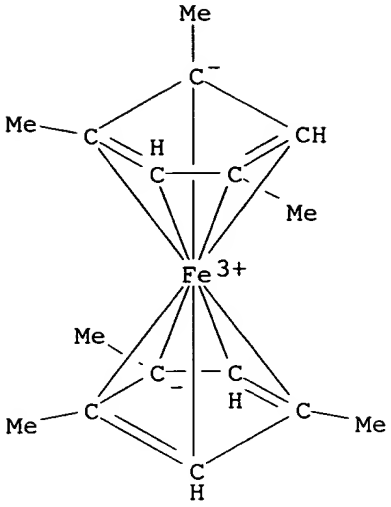

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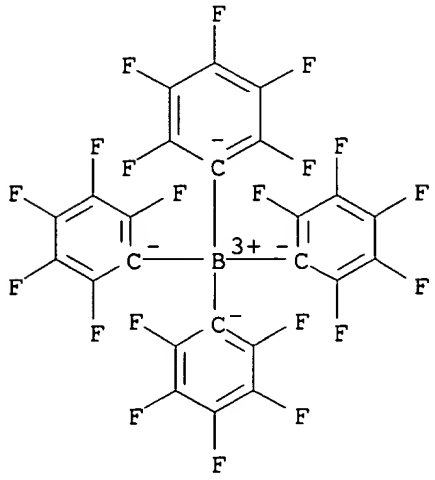

RN 288101-92-8 HCAPLUS
CN Ferrocenium, 1,1',2,2',4,4'-hexamethyl-, tetrakis[4-(trifluoromethyl)phenyl]borate(1-) (9CI) (CA INDEX NAME)

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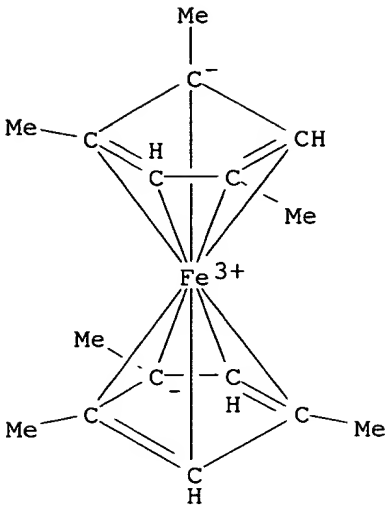
CCI CCS



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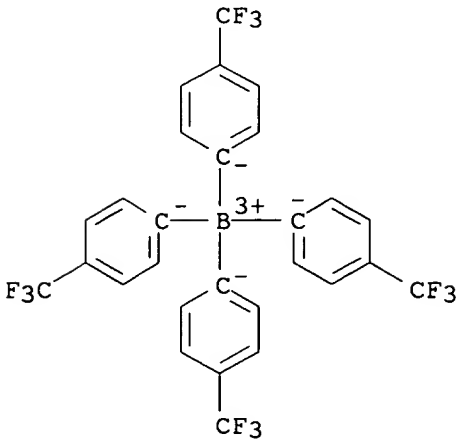

RN 288101-93-9 HCAPLUS
CN Ferrocenium, (2-ferrocenylethyl)-, tetrakis[3,5-bis(trifluoromethyl)phenyl]borate(1-) (9CI) (CA INDEX NAME)

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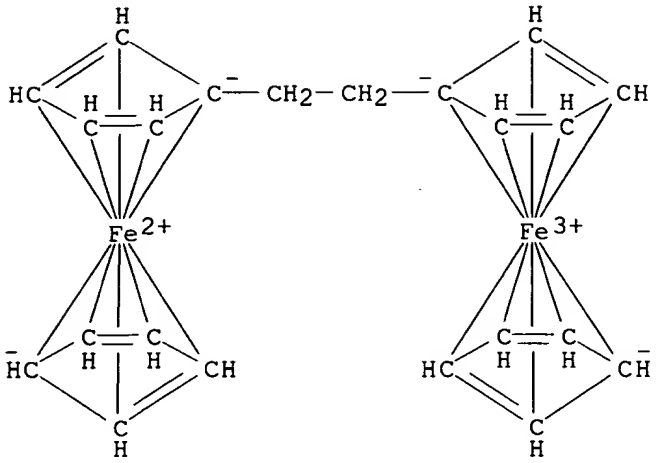
CCI CCS



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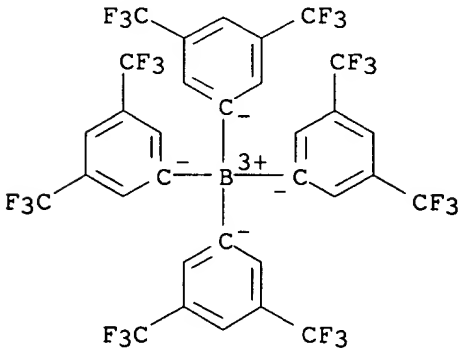

L34 ANSWER 11 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:507131 HCAPLUS
DN 133:252487
ED Entered STN: 27 Jul 2000
TI Bis(Pentafluorophenyl)(2-perfluorobiphenylyl)borane. A New Perfluoroarylborane Cocatalyst for Single-Site Olefin Polymerization
AU Li, Liting; Stern, Charlotte L.; Marks, Tobin J.
CS Department of Chemistry, Northwestern University, Evanston, IL, 60208-3113, USA
SO Organometallics (2000), 19(17), 3332-3337
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-4 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 67, 75

AB Bis(pentafluorophenyl)(2-perfluorobiphenylyl)borane, (C6F5)2B(C12F9) (BPB), was synthesized and characterized to serve as a new strong organo-Lewis acid cocatalyst for single-site olefin polymerization The mol. structure of PBP was determined by x-ray **crystallog**. anal. BPB efficiently activates a variety of Group 4 di-Me complexes to form highly active homogeneous Ziegler-Natta olefin polymerization catalysts. Reaction of BPB with Cp2ZrMe2, rac-Me2Si(Ind)2ZrMe2, and (CGC)MMe2 (M = Zr, Ti; CGC = Me2Si(η5-Me4C5)(tBuN)) (1:1 molar ratio) rapidly and cleanly produces the base-free cationic complexes Cp2ZrMe+[MeB(C12F9)(C6F5)2]- (1), rac-Me2Si(Ind)2ZrMe+[MeB(C12F9)(C6F5)2]- (2), and (CGC)MMe+[MeB(C12F9)(C6F5)2]- (M = Zr, 3; M = Ti, 4), resp. These complexes were characterized by NMR and elemental anal. and are competent for ethylene and propylene polymerization In general, BPB-derived catalysts exhibit polymerization activities comparable to or higher than those of the B(C6F5)3-derived analogs, with the products exhibiting higher mol. wts. but comparable polydispersities, polypropylene isotacticities, and, for ethylene + 1-hexene, comonomer incorporation.

ST fluorophenylfluorobiphenylylborane prepn cocatalyst olefin polymn; borane fluorophenylfluorobiphenylyl prepn cocatalyst olefin polymn; Group IVB dimethylmetal fluorophenylfluorobiphenylylborane catalyst Ziegler Natta olefin polymn; single site olefin polymn fluorophenylfluorobiphenylylboran e cocatalyst; zirconium metallocene olefin polymn catalyst fluorophenylfluorobiphenylylborane cocatalyst; titanium metallocene olefin polymn catalyst fluorophenylfluorobiphenylylborane cocatalyst; metallocene titanium zirconium olefin polymn catalyst fluorophenylfluorobiphenylylbora ne cocatalyst

IT Polymerization catalysts
(Ziegler-Natta; preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)bo rane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin polymerization)

IT Polymerization catalysts
(metallocene; preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)bora ne as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin polymerization)

IT **Crystal** structure
Molecular structure
(of bis(pentafluorophenyl)(perfluorobiphenylyl)borane)

IT Group IVB element complexes
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin polymerization)

IT Polyolefins
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin polymerization)

IT 295367-76-9P, Bis(pentafluorophenyl)(2-perfluorobiphenylyl)borane
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation as cocatalyst with Group 4 dimethylmetal metallocene for olefin polymerization and **crystal** structure of)

IT 9002-88-4P 9003-07-0P 25213-02-9P, Ethylene-1-hexene copolymer 295367-74-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 12636-72-5, Bis(η5-cyclopentadienyl)dimethylzirconium

RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin polymerization)

IT **295367-73-6P** 295367-75-8P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin **polymerization**)

IT 1093-66-9, 2-Perfluorobiphenylyl bromide 2720-03-8, Chlorobis(pentafluorophenyl)borane 135072-62-7 135539-56-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin polymerization)

IT 149197-69-3
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(rac-diastereomer; preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin polymerization)

IT **296230-20-1P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(rac-diastereomer; preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin **polymerization**)

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD

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IT **295367-73-6P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin **polymerization**)

RN 295367-73-6 HCAPLUS
CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, (T-4)-methyl(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)bis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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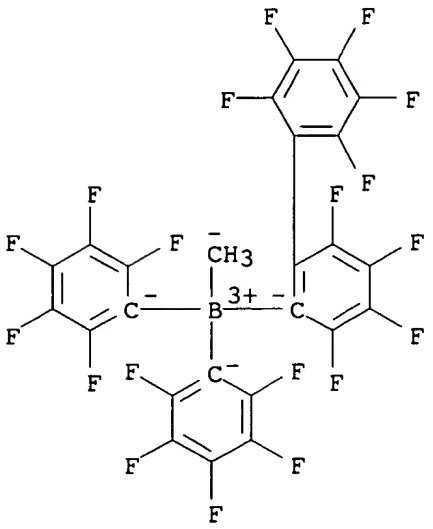
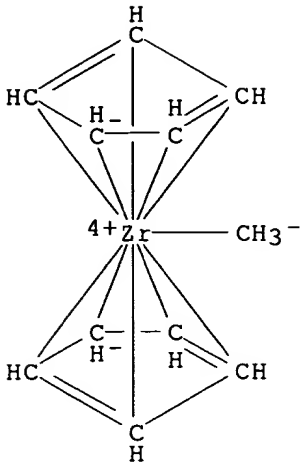
CRN 295367-72-5
CMF C25 H3 B F19
CCI CCS



CM 2

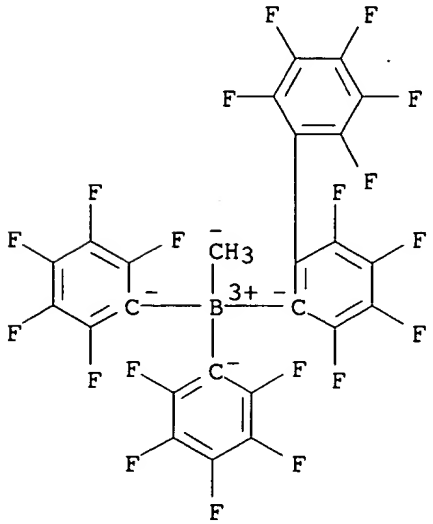
CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS



IT **296230-20-1P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(rac-diastereomer; preparation of bis(pentafluorophenyl)(perfluorobiphenylyl)borane as Lewis acid cocatalyst with Group 4 dimethylmetal for single-site olefin **polymerization**)
RN 296230-20-1 HCAPLUS
CN Zirconium(1+), [(dimethylsilylene)bis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]methyl-, stereoisomer, (T-4)-methyl(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)bis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

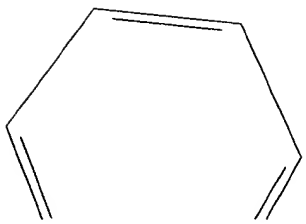
CRN 295367-72-5
CMF C25 H3 B F19
CCI CCS



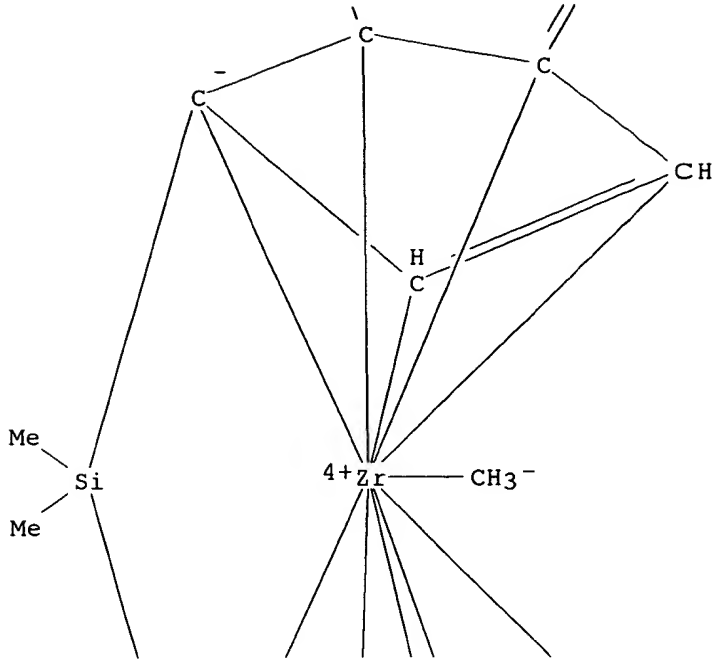
CM 2

CRN 174690-62-1
CMF C21 H21 Si Zr
CCI CCS

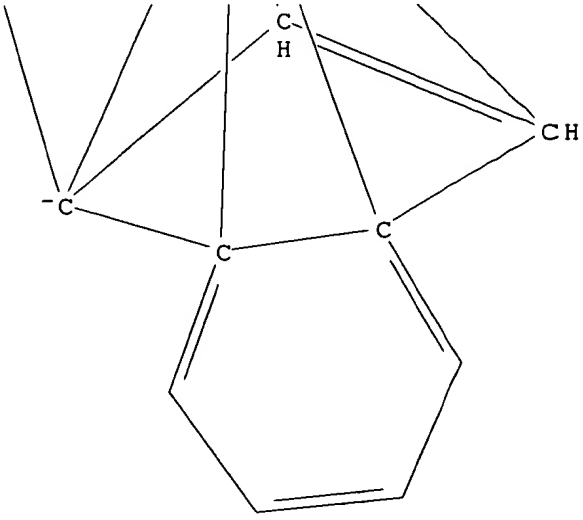
PAGE 1-A



PAGE 2-A



PAGE 3-A



L34 ANSWER 12 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:496850 HCAPLUS
DN 133:252770
ED Entered STN: 24 Jul 2000
TI d0 Metal Olefin Complexes. Synthesis, Structures, and Dynamic Properties of (C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ Complexes: Models for the Elusive

(C5R5)2Zr(R)(Olefin)+ Intermediates in Metallocene-Based Olefin Polymerization Catalysis

AU Carpentier, Jean-Francois; Wu, Zhe; Lee, Chul Woo; Stroemberg, Staffan; Christopher, Joseph N.; Jordan, Richard F.
CS Department of Chemistry, University of Chicago, Chicago, IL, 60637, USA

SO Journal of the American Chemical Society (2000), 122(32), 7750-7767
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29

AB To model the Zr-olefin interaction in the as-yet unobserved (C5R5)2Zr(R)(olefin)+ intermediates in (C5R5)2Zr(R)+-catalyzed olefin polymerization, the coordination of the tethered vinyl group in (C5R5)2Zr(OCMe2(CH2)nCH:CH2)+ species has been investigated. The reaction of (C5H5)2Zr(OCMe2CH2CH2CH:CH2)(Me) with B(C6F5)3 or [Ph3C][B(C6F5)4] yields the chelated olefin complex (C5H5)2Zr(OCMe2CH2CH2CH:CH2)+ as the MeB(C6F5)3- (12a) or B(C6F5)4- (12b) salts. In contrast, the reaction of (C5H5)2Zr(OCMe2CH2CH:CH2)(Me) with B(C6F5)3 in CD2Cl2 yields the MeB(C6F5)3- adduct (C5H5)2Zr(+)(OCMe2CH2CH:CH2)(μ-Me)B(-)(C6F5)3. The reaction of (C5H5)2Zr(OCMe2CH2CH2CH2CH:CH2)(Me) with B(C6F5)3 yields a 1.2/1 mixture (at -90 °C) of the chelated olefin complex (C5H5)2Zr(OCMe2CH2CH2CH2CH:CH2)+ and the MeB(C6F5)3- adduct (C5H5)2Zr(+)(OCMe2CH2CH2CH:CH2)(μ-Me)B(-)(C6F5)3'. The reaction of rac-(EBI)Zr(OCMe2CH2CH2CH:CH2)(Me) (EBI = ethylene-1,2-bis(1-indenyl)) with B(C6F5)3 or [Ph3C][B(C6F5)4] yields the chelated olefin complex rac-(EBI)Zr(OCMe2CH2CH2CH:CH2)+ as the MeB(C6F5)3- (20a) or B(C6F5)4- (20b) salts, each as a 1/1 mixture of diastereomers which differ in the relative configuration of the rac-(EBI)Zr unit and the internal carbon of the coordinated olefin. X-ray diffraction analyses of 12a and the S,S,R/R,R,S isomer of 20a, and NMR data for 12a,b and 20a,b establish that the Zr-olefin bonding in these species is unsym. and consists of a weak Zr-Cterm interaction and minimal Zr-Cint interaction (12a, Zr-Cterm = 2.68(2), Zr-Cint = 2.89(2) Å; 20a, Zr-Cterm = 2.634(5), Zr-Cint = 2.819(4) Å). X-ray (dC:C), IR (νC:C), and NMR (1H, 13C) data show that the Zr-olefin interaction does not significantly perturb the structure of the coordinated olefin but does polarize the C:C bond such that pos. charge buildup occurs at Cint. Similar unsym. bonding and polarization effects may contribute to the high insertion reactivity of (C5R5)2Zr(R)(α-olefin)+ species. Dynamic NMR studies show that 12a,b and 20a,b undergo olefin face exchange in solution on the NMR time scale. The free energy barrier for face exchange of 20a (ΔG.thermod.FE = 15.4(4) kcal/mol at 43 °C) is significantly greater than that for 12a (ΔG.thermod.FE = 10.7(5) kcal/mol at -55 °C). Possible origins of this difference are discussed. The face exchange of 20a is dissociative, with minimal involvement of anion, solvent, or σ-complex intermediates.

ST zirconium indenyl cyclopentadienyl olefin complex synthesis model polymn catalyst; olefin face exchange free energy zirconium complex

IT Bond angle
Bond length
Crystal structure
Molecular structure
Polymerization catalysts
Substitution reaction, coordinative
(synthesis, structures, and dynamic properties of (C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for

(C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin polymerization
catalysis)
IT Transition metal complexes
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(synthesis, structures, and dynamic properties of
(C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for
(C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin polymerization
catalysis)
IT Polyolefins
RL: MSC (Miscellaneous)
(synthesis, structures, and dynamic properties of
(C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for
(C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin polymerization
catalysis)
IT 294636-75-2P **294636-79-6P 294638-90-7P**
294638-91-8P 294638-96-3P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(synthesis, structures, and dynamic properties of
(C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for
(C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin **polymerization** catalysis)
IT 60-29-7, Diethyl ether, reactions 109-49-9, 5-Hexen-2-one 109-99-9, reactions 624-97-5, 2-Methyl-4-penten-2-ol 917-54-4, Methyllithium 1109-15-5, Tris(pentafluorophenyl)boron 1119-51-3 12636-72-5, Dimethylzirconocene 23616-79-7, Tributylbenzylammonium chloride 136040-19-2, Triphenylcarbenium tetrakis(pentafluorophenyl)borate 136844-77-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis, structures, and dynamic properties of
(C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for
(C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin polymerization
catalysis)
IT 16744-89-1P, 2-Methyl-5-hexen-2-ol 70083-57-7P, Lithium Methyltris(pentafluorophenyl)borate 77437-98-0P, 2-Methyl-6-hepten-2-ol 166544-85-0P 166544-86-1P 166544-87-2P 166987-10-6P 294636-70-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis, structures, and dynamic properties of
(C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for
(C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin polymerization
catalysis)
IT 166544-91-8P 166544-94-1P 166987-11-7P 166987-12-8P 166987-13-9P 166987-14-0P 293736-17-1P 294636-72-9P 294636-82-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis, structures, and dynamic properties of
(C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for
(C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin polymerization
catalysis)
RE.CNT 160 THERE ARE 160 CITED REFERENCES AVAILABLE FOR THIS RECORD
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IT **294636-79-6P 294638-90-7P 294638-91-8P 294638-96-3P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(synthesis, structures, and dynamic properties of (C5R5)2Zr(OCMe2CH2CH2CH:CH2)+ complexes as models for (C5R5)2Zr(R)(Olefin)+ intermediates in metallocene-based olefin **polymerization** catalysis)

RN 294636-79-6 HCAPLUS

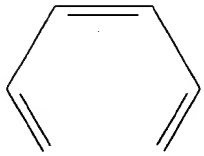
CN Zirconium(1+), [1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]][(5,6-η)-2-methyl-5-hexen-2-olato-κO]-, stereoisomer,

(T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 294636-78-5
CMF C27 H29 O Zr
CCI CCS

PAGE 1-A



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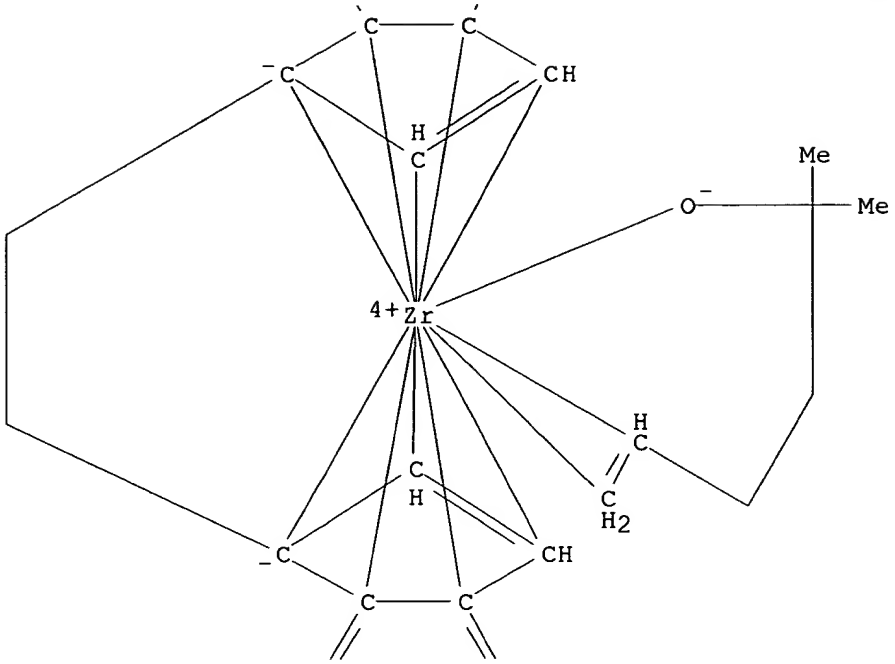

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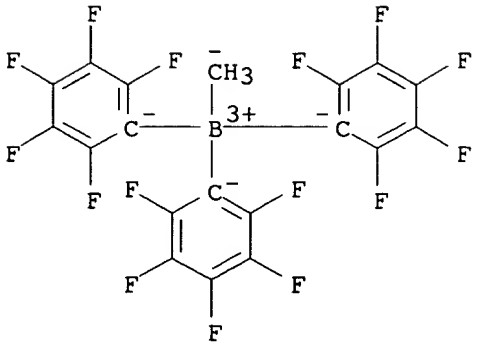
CCI CCS



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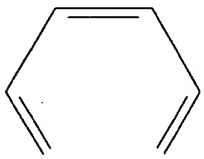
CM 1

CRN 294638-89-4
CMF C27 H29 O Zr
CCI CCS

PAGE 1-A



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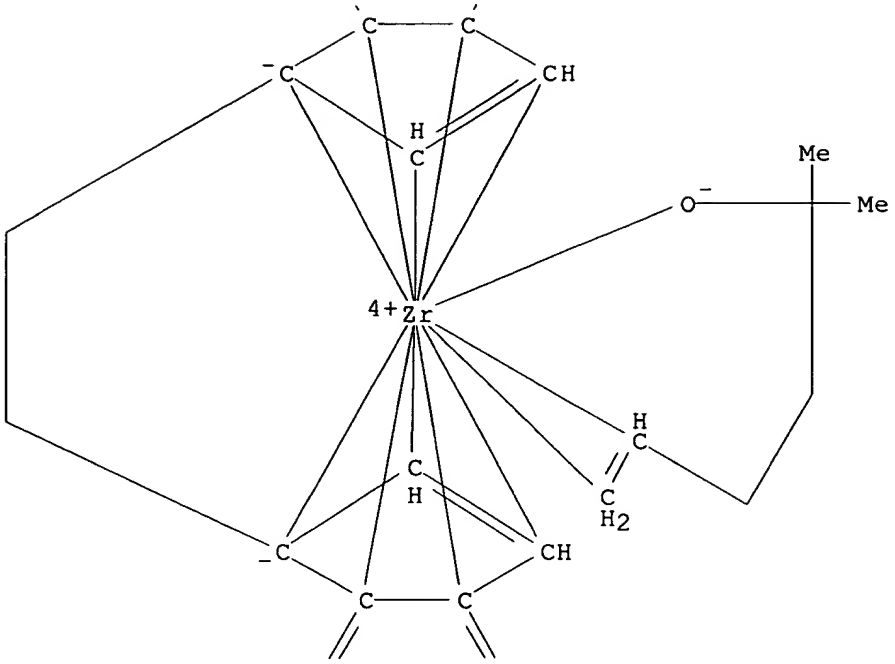

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CM 2

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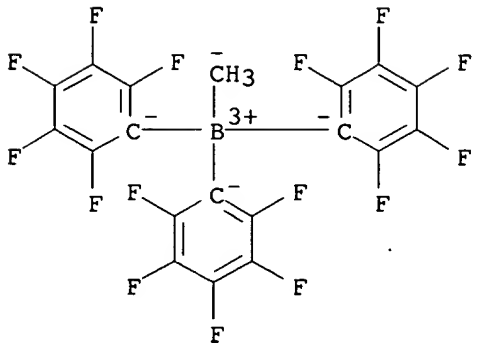
CCI CCS

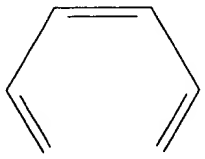


RN 294638-91-8 HCAPLUS
CN Zirconium(1+), [1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]][(5,6-η)-2-methyl-5-hexen-2-olato-κO]-, stereoisomer, (T-4)-tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 294638-89-4
CMF C27 H29 O Zr
CCI CCS

PAGE 1-A



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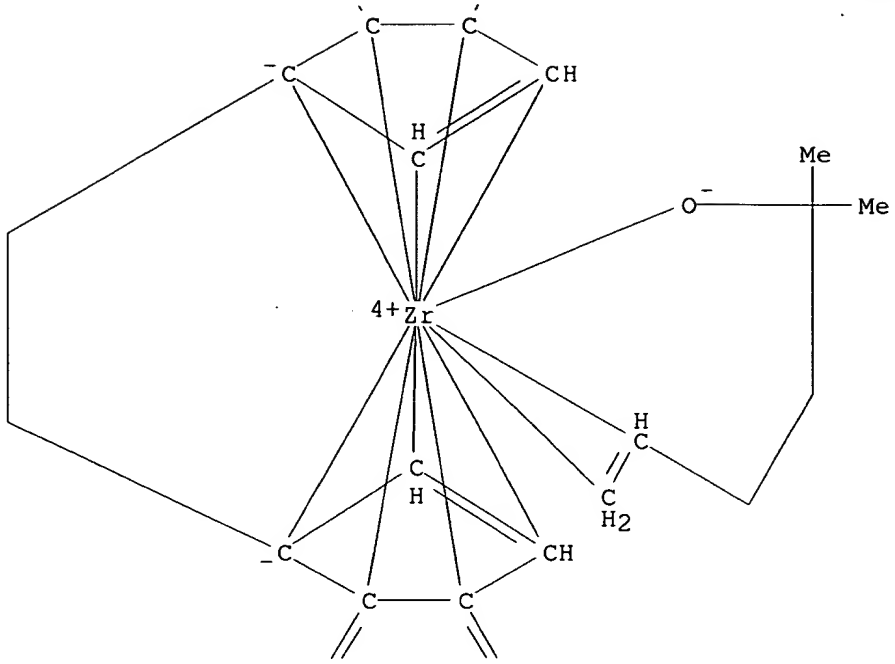

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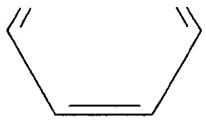

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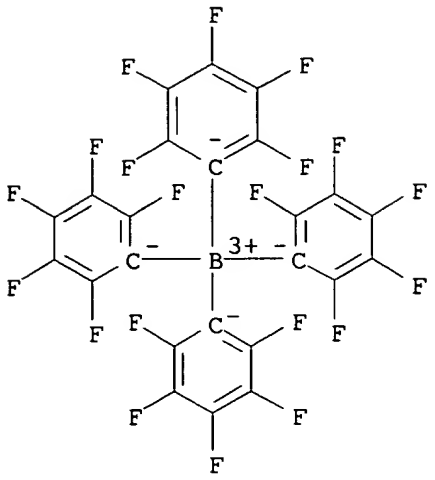
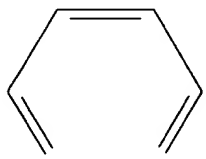
CCI CCS



RN 294638-96-3 HCAPLUS
CN Zirconium(1+), [1,2-ethanediylbis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]][(5,6-η)-2-methyl-5-hexen-2-olato-κO]-, stereoisomer, (T-4)-tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 294636-78-5
CMF C27 H29 O Zr
CCI CCS



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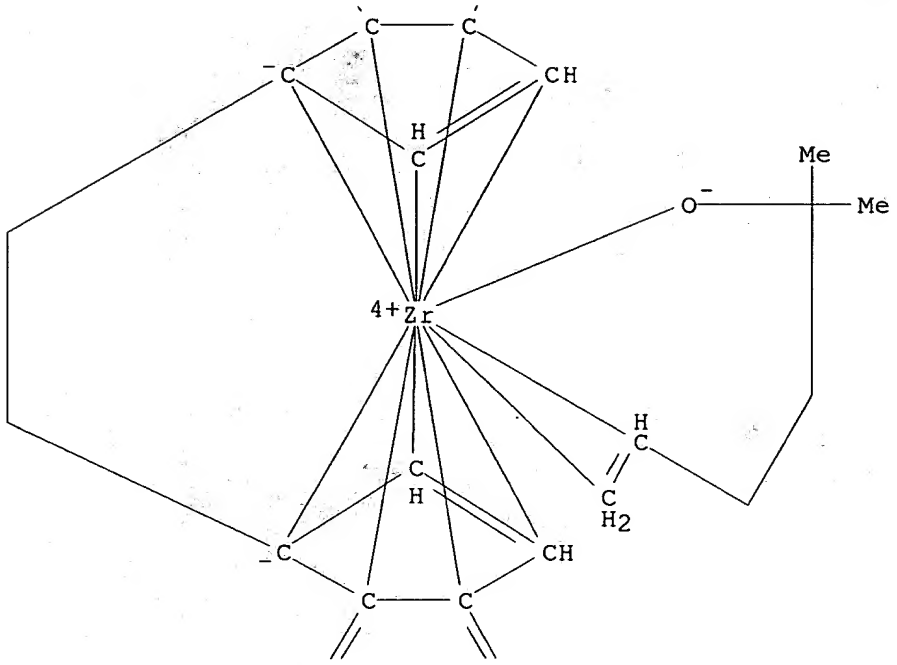

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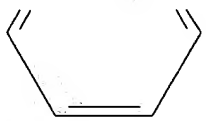

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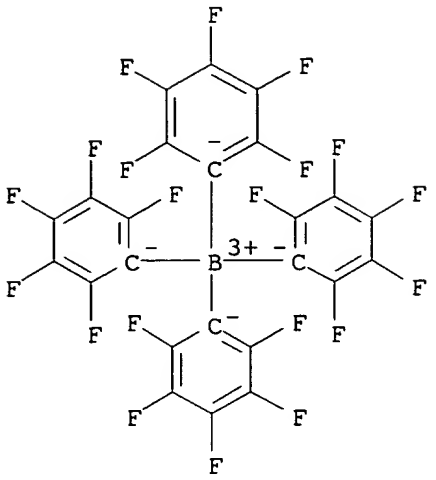

L34 ANSWER 13 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:437901 HCAPLUS
DN 133:193224
ED Entered STN: 30 Jun 2000
TI Structural Dichotomy in Single-Component Ziegler Catalyst Systems: Characterization of Zr···F and Zr···C-Bonded Structural Types of Group 4 Metallocene [C4H6-B(C6F5)3] Betaines
AU Dahlmann, Marc; Erker, Gerhard; Froehlich, Roland; Meyer, Oliver
CS Organisch-Chemisches Institut, Universitaet Muenster, Muenster, D-48149, Germany
SO Organometallics (2000), 19(16), 2956-2967
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 35, 75
AB The organometallic Lewis acid B(C6F5)3 adds to the terminal :CH2 group of the (butadiene)metallocene complexes to give the ansa-metallocene betaine systems [Me2Si(C5H4)2]Zr[C4H6-B(C6F5)3] (6a) and [Me2Si(3-MeC5H3)2]Zr[C4H6-B(C6F5)3] (6b) in high yield. Both complexes were characterized by x-ray diffraction. They both contain a substituted η3-allyl ligand F of E configuration, and they show a characteristic (ortho aryl)C-F···Zr interaction that stabilizes the electron-deficient metal center inside the dipolar structure. B(C6F5)3 also adds to one butadiene terminus of (s-cis-η4-C4H6)[Me2C(C5H4)(indenyl)]Zr to give a high yield of a single isomer of the resp. ansa-metallocene [C4H6-B(C6F5)3] betaine complex 9. The x-ray **crystal** structure anal. of 9 has revealed that in this case a (Z)-η3-allyl-CH2B(C6F5)3 ligand is formed. This precluded the (aryl)C-F···Zr coordination. Instead, the zirconium center in 9 forms a stabilizing internal ion pair interaction between the neg. polarized [B]-C(4)H2 methylene group and the pos. zirconium center. The analogously structured ansa-metallocene [(Z)-C4H6-B(C6F5)3] betaine complex 12 is obtained in high yield from B(C6F5)3 addition to (s-cis-η4-butadiene)[Me2C(C5H4)(fluorenyl)]Zr. In solution the complexes

6, 9, and 12 exhibit structures that are analogous to those found in the solid state. However, treatment of (butadiene)[Me2Si(C5H4)2]Zr with B(C6F5)3 under kinetic control (233 K in toluene-d8) quant. yields the [Me2Si(C5H4)2]Zr[(Z)-C4H6-B(C6F5)3] betaine isomer 13, which contains the stabilizing [B]-C(4)H2···Zr internal ion pair interaction. Subsequent thermally induced rearrangement of the kinetic product 13 (ΔG.thermod.rearr(298 K) = 21.5 ± 0.5 kcal mol-1) then results in the formation of the eventually observed thermodn. ansa-metallocene betaine product 6a, that contains the (E)-C4H6-B(C6F5)3 ligand and exhibits internal (aryl)C-F···Zr coordination. A similar reaction sequence was observed during the addition of B(C6F5)3 to the parent (butadiene)zirconocene system: at 213 K the kinetic Cp2Zr[(Z)-(1-3η),κC4-C4H6-B(C6F5)3] betaine product is formed, which rapidly rearranges at temps. above 253 K to yield the previously observed stable Cp2Zr[(E)-C4H6-B(C6F5)3] betaine system, which is characterized by an internal C-F···Zr bond. The ansa-metallocene betaines 6, 9, and 12 are all active homogeneous single-component Ziegler catalysts for ethene and propene polymerization They are similarly effective as the usually employed ansa-metallocene dichloride/methylalumoxane catalyst systems.

ST ansa zirconocene betaine complex prepn Ziegler catalyst olefin polymn; **crystal** mol structure ansa zirconocene betaine complex; butadiene zirconocene prepn reaction fluorophenyl borane

IT Aluminoxanes
RL: CAT (Catalyst use); USES (Uses)
(Me; preparation of ansa zirconocene butadiene and betaine complexes as polymerization catalysts in presence of)

IT **Crystal** structure
Molecular structure
(of ansa zirconocene butadiene and betaine complexes)

IT Polymerization catalysts
(preparation of ansa zirconocene butadiene and betaine complexes as)

IT 130638-44-7 133518-41-9
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(olefin polymerization catalytic activity and reaction with butadiene magnesium)

IT 289056-50-4P 289056-53-7P 289056-57-1P 289057-08-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and **crystal** structure of)

IT 289056-54-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and rearrangement of)

IT 9002-88-4P 9003-07-0P, Polypropylene 171003-33-1P 289056-55-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **289056-52-6P** 289056-56-0P
RL: **CAT (Catalyst use)**; PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation, mol. structure, and olefin **polymerization** catalytic activity of)

IT **289056-49-1P**
RL: **CAT (Catalyst use)**; PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation, olefin **polymerization** catalytic activity, and mol. structure of)

IT 158111-56-9P 289056-47-9P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, olefin polymerization catalytic activity, and reaction with tris(pentafluorophenyl)borane)

IT 289056-51-5P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, olefin polymerization catalytic activity, reaction with tris(pentafluorophenyl)borane)

IT 289056-48-0P
RL: CAT (Catalyst use); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, olefin polymerization catalytic activity, reaction with tris(pentafluorophenyl)borane, and **crystal** structure of)

IT 86050-32-0, Dichloro(dimethylsilylenebis(η5-cyclopentadienylidene))zirconium 158051-88-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with butadiene magnesium)

IT 1109-15-5, Tris(pentafluorophenyl)borane 70809-00-6, Butadiene magnesium
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with butadiene zirconocene complexes)

IT 83780-93-2 83780-95-4 250638-65-4 250663-12-8 250663-34-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with tris(pentafluorophenyl)borane)

RE.CNT 131 THERE ARE 131 CITED REFERENCES AVAILABLE FOR THIS RECORD

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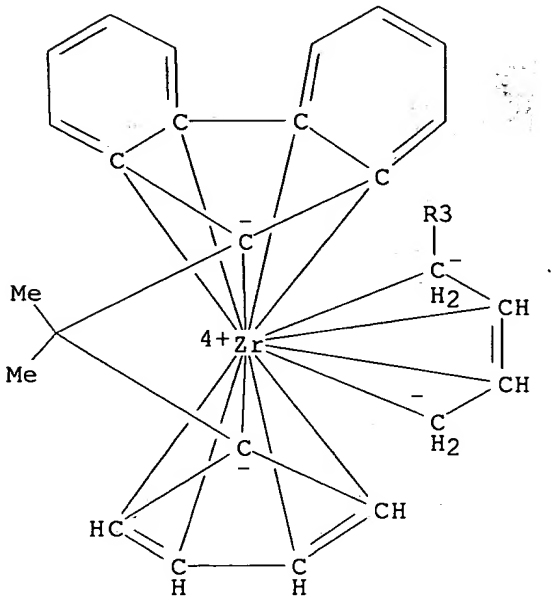
IT **289056-52-6P**
RL: **CAT (Catalyst use)**; PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation, mol. structure, and olefin **polymerization** catalytic activity of)

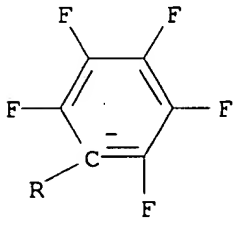
RN 289056-52-6 HCAPLUS

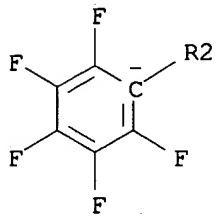
CN Zirconium, [μ-[(1-η:1,2,3,4-η)-(2Z)-2-butene-1,4-diyl]][η10-2,4-cyclopentadien-1-ylidene(1-methylethylidene)-9H-fluoren-9-ylidene][tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A





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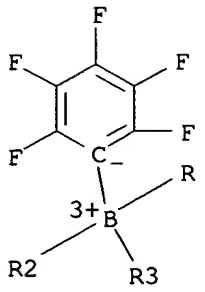
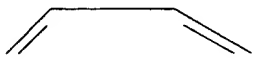


IT **289056-49-1P**
RL: **CAT (Catalyst use)**; PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation, olefin **polymerization** catalytic activity, and mol. structure of)
RN 289056-49-1 HCAPLUS
CN Zirconium, [μ-[(1-η:1,2,3,4-η)-(2Z)-2-butene-1,4-diyl]][η10-2,4-cyclopentadien-1-ylidene(1-methylethylidene)-1H-inden-1-ylidene][tris(pentafluorophenyl)boron]-, stereoisomer (9CI) (CA INDEX NAME)

PAGE 1-A



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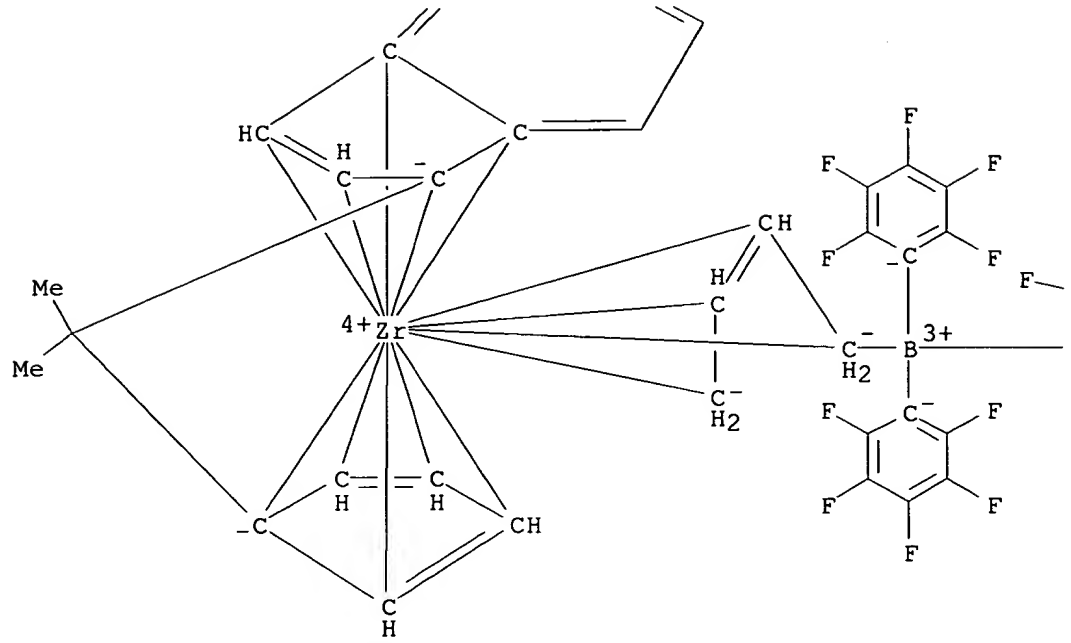

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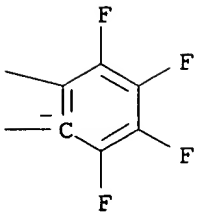

L34 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:84010 HCAPLUS
DN 132:237402
ED Entered STN: 04 Feb 2000
TI Silica-Grafted Borato Cocatalysts for Olefin Polymerization Modeled by Silsesquioxane-Borato Complexes
AU Duchateau, Robbert; Van Santen, Rutger A.; Yap, G. P. A.
CS Dutch Polymer Institute/Schuit Institute of Catalysis, Eindhoven University of Technology, Eindhoven, 5600 MB, Neth.
SO Organometallics (2000), 19(5), 809-816
CODEN: ORGND7; ISSN: 0276-7333

PB American Chemical Society
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29
AB The syntheses and reactivity studies of silsesquioxane-borato complexes are described. Treatment of B(C6F5)3 with (c-C5H9)7Si8O12(OH) and (c-C5H9)7Si7O9(OH)3 in the presence of a Bronsted base yields the silsesquioxane-borates X+{[(c-C5H9)7Si8O13]B(C6F5)3}- (1a, X+ = PhN(H)Me2+; 1b, X+ = Et3NH+) and X+{[(c-C5H9)7Si7(OH)2O10]B(C6F5)3}- (1b, X+ = PhN(H)Me2+; 2b, X+ = Et3NH+), resp. When the more nucleophilic base pyridine is used, (C6F5)3B·NC5H5 (3) is formed instead, demonstrating the competition between B(C6F5)3 and H+ to react with the amine. The dimethylaniline in 1a and 2a is readily exchanged by NEt3 to form 1b and 2b. With the nucleophilic Lewis base NC5H5, the B-O bond in 1a and 2a is split, yielding (C6F5)3B·NC5H5 (3) and the free silsesquioxanes. Complexes 1 and 2 rapidly undergo hydrolysis under formation of the hydroxyl complexes X+{(C6F5)3BOH}- (4a, X+ = PhN(H)Me2+; 4b, X+ = Et3NH+). Likewise, alcoholysis of 1a and 2a with i-PrOH yields the alkoxide {PhN(H)Me2}+{i-PrOB(C6F5)3}- (5). The B-O bond is only moderately stable toward early-transition-metal alkyls. Nevertheless, Cp2Zr(CH2Ph)2 + 1a and Zr(CH2Ph)4 + 2a form single-site ethylene polymerization catalysts. Detailed reactivity studies demonstrated that both B-O and B-C bond splitting plays a crucial role, as not 1a and 2a, but their decomposition product B(C6F5)3 is the actual cocatalyst. The solid-state structures of 1a and 4b were determined by single-**crystal** X-ray anal.
ST silica boron cocatalyst olefin polymn silsesquioxane model
IT Silsesquioxanes
RL: CAT (Catalyst use); USES (Uses)
(borate complexes; silica-grafted borato cocatalysts for olefin polymerization
modeled by silsesquioxane-borato complexes)
IT **Crystal** structure
Polymerization catalysts
(silica-grafted borato cocatalysts for olefin polymerization modeled by silsesquioxane-borato complexes)
IT Bases, uses
RL: CAT (Catalyst use); USES (Uses)
(silica-grafted borato cocatalysts for olefin polymerization modeled by silsesquioxane-borato complexes)
IT 24356-01-2, Tetrabenzylzirconium 262300-71-0
RL: CAT (Catalyst use); USES (Uses)
(catalyst precursor; silica-grafted borato cocatalysts for olefin polymerization modeled by silsesquioxane-borato complexes)
IT 37206-41-0
RL: CAT (Catalyst use); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(catalyst precursor; silica-grafted borato cocatalysts for olefin polymerization modeled by silsesquioxane-borato complexes)
IT 262300-66-3P 262300-73-2P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(copy; silica-grafted borato cocatalysts for olefin polymerization modeled by
silsesquioxane-borato complexes)
IT 2138-72-9 7631-86-9, Silica, uses
RL: CAT (Catalyst use); USES (Uses)
(silica-grafted borato cocatalysts for olefin polymerization modeled by

silsesquioxane-borato complexes)
IT 262300-64-1P 262300-72-1P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(silica-grafted borato cocatalysts for olefin polymerization modeled by silsesquioxane-borato complexes)
IT 262300-67-4P **262300-69-6P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(silica-grafted borato cocatalysts for olefin **polymerization** modeled by silsesquioxane-borato complexes)
IT 110-86-1, Pyridine, reactions 121-44-8, reactions 121-69-7, Dimethylphenylamine, reactions 1109-15-5, Tris(pentafluorophenyl)boron 183387-28-2 216972-58-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(silica-grafted borato cocatalysts for olefin polymerization modeled by silsesquioxane-borato complexes)
IT 9002-88-4P, Polyethylene 147892-18-0P 262300-74-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(silica-grafted borato cocatalysts for olefin polymerization modeled by silsesquioxane-borato complexes)
RE.CNT 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD
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IT **262300-69-6P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(silica-grafted borato cocatalysts for olefin **polymerization** modeled by silsesquioxane-borato complexes)

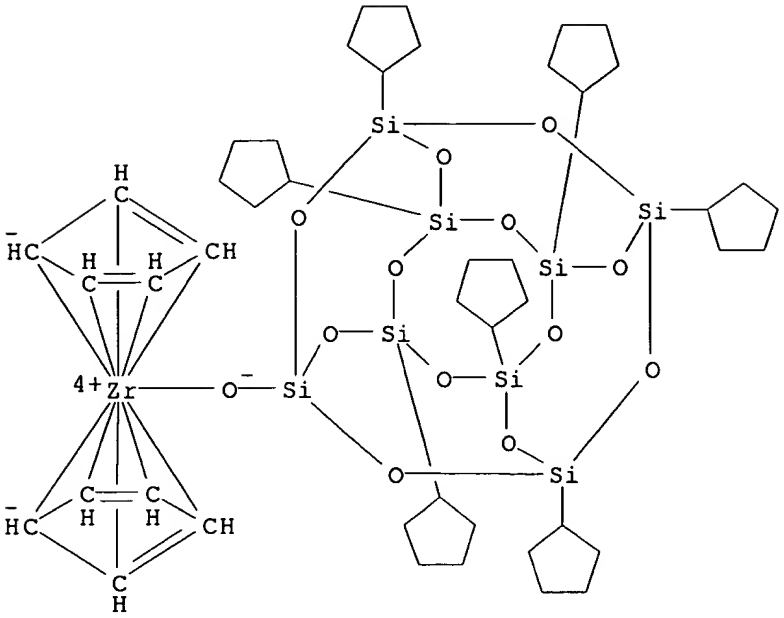
RN 262300-69-6 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)(heptacyclopentylpentacyclo[9.5.1.13,9.15,15.17,13]octasiloxanolato-κO1)-, (T-4)-tris(pentafluorophenyl)(phenylmethyl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

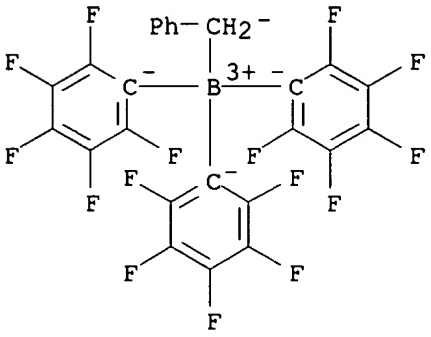
CRN 262300-68-5

CMF C45 H73 O13 Si8 Zr
CCI CCS



CM 2

CRN 149831-05-0
CMF C25 H7 B F15
CCI CCS



L34 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2000:81709 HCAPLUS
DN 132:222593
ED Entered STN: 03 Feb 2000
TI (N-pyrrolyl)B(C6F5)2-a new organometallic Lewis acid for the generation of Group 4 metallocene cation complexes
AU Kehr, Gerald; Frohlich, Roland; Wibbeling, Birgit; Erker, Gerhard
CS Organisch-Chemisches Institut der Universitat, Munster, D-48149, Germany

SO Chemistry--A European Journal (2000), 6(2), 258-266
CODEN: CEUJED; ISSN: 0947-6539
PB Wiley-VCH Verlag GmbH
DT Journal
LA English
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35, 75

AB Treatment of the (C6F5)2BF·OEt2 (3) complex with N-pyrrolyl Li gives bis(pentafluorophenyl)(N-pyrrolyl)borane (2), a strong organometallic Lewis acid, which was characterized by x-ray diffraction (B-N bond length: 1.401(5) Å). It exhibits a columnar superstructure in the **crystal** and contains π-stacks of pyrrolyl units. Compound 2 readily abstrs. alkyl anions from a variety of alkyl Group 4 metallocene-type complexes and leads to the clean formation of the resp. metallocene ions or ion pairs. For example, the treatment of Cp3ZrCH3 (9) with 2 transfers a Me anion to yield the ion pair [Cp3Zr]+[(C4H4N)BMe(C6F5)2]- (12). The x-ray **crystal** structure anal. of 12 shows a close contact between Zr and the pyrrolyl-β-C (2.641(2) Å). The borane 2 adds to (butadiene)zirconocene (13) to yield the betaine system [Cp2Zr]+[(H2C:CHCHCH2)B(NC4H4)(C6F5)2]- (15). Complex 15 contains a distorted η3-allyl moiety inside the metallacyclic framework and it features an internal Zr+···(pyrrolyl)B- ion pair interaction with a Zr···pyrrolyl-α-C separation of 2.723(3) Å (determined by x-ray diffraction). From the dynamic NMR spectra of 15 the bond strength of the internal ion pair interaction is ΔG.thermod.diss (223 K) ≈15 kcal mol-1. Treatment of dimethylzirconocene (16) with 2 yields the metallocene borate salt [Cp2ZrCH3]+[(C4H4N)BMe(C6F5)2]- (17), which is an active catalyst for the polymerization of ethene.

ST **crystal** structure pyrrolylborane pyrrolidinylborane zirconocene pyrrolylborate ion pair betaine; mol structure pyrrolylborane pyrrolidinylborane zirconocene pyrrolylborate ion pair betaine; ethene polymn catalyst zirconocene pyrrolylborate; pyrrolylborane prepn structure reaction zirconocene; borane pyrrolyl pyrrolidinyl prepn structure; zirconocene methyl butadiene complex reaction pyrrolylborane; ion pair zirconocene pyrrolylborate prepn structure; betaine zirconocene pyrrolylborate prepn structure; bond strength ion pair zirconocene pyrrolylborate

IT Dissociation enthalpy
(of betaine derived from zirconium butadiene and pyrrolyldiarylborane)

IT **Crystal** structure
Molecular structure
(of pyrrolyldiarylborane, pyrrolidinyldiarylborane, zirconium cyclopentadienyl methyl(pyrrolyl)diarylborate ion pair, and betaine derived from zirconium butadiene and pyrrolyldiarylborane)

IT Free energy of activation
(of rotation about boron-aryl bond and of dissociation of zirconocene betaine and zirconocene Me complex borates)

IT Ion pairs
(preparation and dissociation barriers of zirconocene Me complex borates)

IT Polymerization catalysts
(zirconocene Me methyl(pyrrolyl)bis(pentafluorophenyl)borate for ethylene)

IT 1109-15-5, Tris(pentafluorophenyl)borane
RL: RCT (Reactant); RACT (Reactant or reagent)
(Me anion transfer reaction with zirconium cyclopentadienyl Me complex)

IT 12636-72-5, Bis(η5-cyclopentadienyl)dimethylzirconium 75374-50-4, (η4-1,3-Butadiene)bis(η5-cyclopentadienyl)zirconium 185549-24-0,

Tris(η5-cyclopentadienyl)(methyl)zirconium
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbanion transfer reaction with diaryl(pyrrolyl)borane)
IT 68193-38-4, Dimethylbis(η5-methylcyclopentadienyl)zirconium
RL: RCT (Reactant); RACT (Reactant or reagent)
(carbanion transfer reactions with diaryl(pyrrolyl)borane and triarylborane)
IT 100-99-2, Triisobutyl aluminum, uses
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst for ethylene polymerization)
IT 109-97-7, Pyrrole
RL: RCT (Reactant); RACT (Reactant or reagent)
(lithiation followed by metathesis with fluorodiarylborane-ether adduct)
IT 71312-71-5, Dichloro(N-pyrrolidinyl)borane
RL: RCT (Reactant); RACT (Reactant or reagent)
(metathesis with aryllithium)
IT 1076-44-4, (Pentafluorophenyl)lithium
RL: RCT (Reactant); RACT (Reactant or reagent)
(metathesis with chloro(pyrrolidinyl)borane)
IT 4439-90-1, Lithium pyrrolidide
RL: RCT (Reactant); RACT (Reactant or reagent)
(metathesis with fluorodiarylborane-ether adduct)
IT 197009-46-4, (Diethyl ether)(fluoro)bis(pentafluorophenyl)boron
RL: RCT (Reactant); RACT (Reactant or reagent)
(metathesis with lithiated pyrrole and pyrrolidine)
IT **261376-52-7P**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) methylbis(pentafluorophenyl)(N-pyrrolyl)borate
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and catalysis of **polymerization** of ethylene by)
IT 261347-74-4P, Bis(pentafluorophenyl)(N-pyrrolidinyl)borane 261347-81-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and **crystal** structure of)
IT 261347-95-9P, Methylbis(η5-methylcyclopentadienyl)zirconium(1+) methyltris(pentafluorophenyl)borate(1-) 261376-54-9P, Methylbis(η5-methylcyclopentadienyl)zirconium(1+) methylbis(pentafluorophenyl)(N-pyrrolyl)borate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and ion-pair dissociation barrier of)
IT 261347-75-5P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mol. structure of)
IT 9002-88-4P, Polyethylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 261347-73-3P, Bis(pentafluorophenyl)(N-pyrrolyl)borane
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, **crystal** structure and carbanion transfer reactions with zirconium cyclopentadienyl Me and butadiene complexes)
IT 261347-76-6P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation, **crystal** structure and rotational and dissociation barrier of)
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
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IT **261376-52-7P**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) methylbis(pentafluorophenyl)(N-pyrrolyl)borate
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and catalysis of **polymerization** of ethylene by)

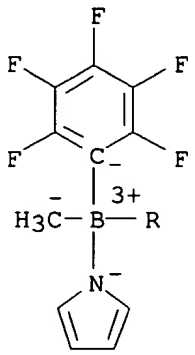
RN 261376-52-7 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, (T-4)-methylbis(pentafluorophenyl)-1H-pyrrol-1-ylborate(1-) (9CI) (CA INDEX NAME)

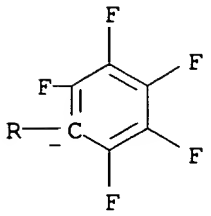
CM 1

CRN 261376-51-6
CMF C17 H7 B F10 N
CCI CCS

PAGE 1-A



PAGE 2-A



CM 2

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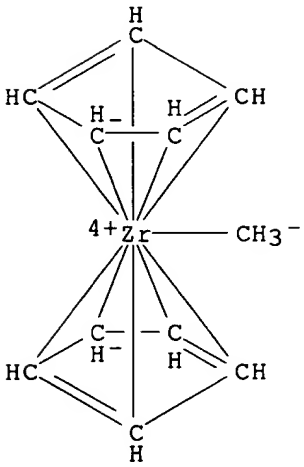
CCI CCS



L34 ANSWER 16 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:113689 HCAPLUS
DN 130:182880
ED Entered STN: 19 Feb 1999
TI Activators for transition metal complex catalysts for polymerization of olefins
IN Mcadon, Mark H.; Nickias, Peter N.; Marks, Tobin J.; Swartz, David J.
PA The Dow Chemical Company, USA; Northwestern University
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07F005-02
ICS C08F010-00
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

PI WO 9906413 A1 19990211 WO 1998-US14106 19980707
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG
AU 9887572 A1 19990222 AU 1998-87572 19980707
EP 1000069 A1 20000517 EP 1998-939073 19980707
EP 1000069 B1 20030312
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, LU, SE, FI
BR 9810123 A 20000808 BR 1998-10123 19980707
JP 2001512127 T2 20010821 JP 2000-505171 19980707
AT 234311 E 20030315 AT 1998-939073 19980707
US 6268445 B1 20010731 US 1999-424277 19991119
NO 9906176 A 19991214 NO 1999-6176 19991214
MX 9912042 A 20000930 MX 1999-12042 19991217
PRAI US 1997-54586P P 19970801
WO 1998-US14106 W 19980707
OS MARPAT 130:182880
AB A catalyst activator particularly adapted for use in the activation of metal complexes of metals of Group 3-10 for polymerization of ethylenically unsatd. polymerizable monomers, especially olefins, comprises two Group 13 metal or metalloid atoms and a ligand structure including at least one bridging group connecting ligands on the two Group 13 metal or metalloid atoms. A typical activator was manufactured by heating 1.26 mmol 1,4-C6F4(SnMe3)2 with (C6F4)2BCl 72 h at 140° under 0.1 torr pressure.
ST activator transition metal complex catalyst olefin polymn; fluorophenylene fluorophenylborane activator transition metal complex polymn catalyst
IT Polymerization catalysts
(activators for transition metal complex catalysts for polymerization of olefins)
IT Group IIIA element compounds
Lewis acids
RL: CAT (Catalyst use); USES (Uses)
(activators for transition metal complex catalysts for polymerization of olefins)
IT Polyolefins
RL: IMF (Industrial manufacture); PREP (Preparation)
(activators for transition metal complex catalysts for polymerization of olefins)
IT 220503-32-2P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(activator precursor; activators for transition metal complex catalysts for polymerization of olefins)
IT 2720-03-8 10294-34-5, Boron trichloride 12636-72-5, Bis(cyclopentadienyl)dimethylzirconium 23653-79-4 23653-80-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(activator precursor; activators for transition metal complex catalysts for polymerization of olefins)
IT 135072-62-7
RL: CAT (Catalyst use); USES (Uses)
(activators for transition metal complex catalysts for polymerization of olefins)

IT 200009-41-2P 220503-31-1P 220503-33-3P **220503-35-5P**
220503-37-7P 220503-40-2P 220503-42-4P
RL: **CAT (Catalyst use)**; IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(activators for transition metal complex catalysts for **polymn**. of olefins)

IT 9003-07-0P
RL: IMF (Industrial manufacture); PREP (Preparation)
(activators for transition metal complex catalysts for polymerization of olefins)

IT 220503-38-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and **crystal** structure of)

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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(17) Spence, R; Organometallics 1998, V17(12), P2459 HCAPLUS

IT **220503-35-5P 220503-37-7P**
RL: **CAT (Catalyst use)**; IMF (Industrial manufacture); PREP (Preparation); USES (Uses)
(activators for transition metal complex catalysts for **polymn**. of olefins)

RN 220503-35-5 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, (T-4)-[4-[bis(pentafluorophenyl)boryl]-2,3,5,6-tetrafluorophenyl]methylbis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

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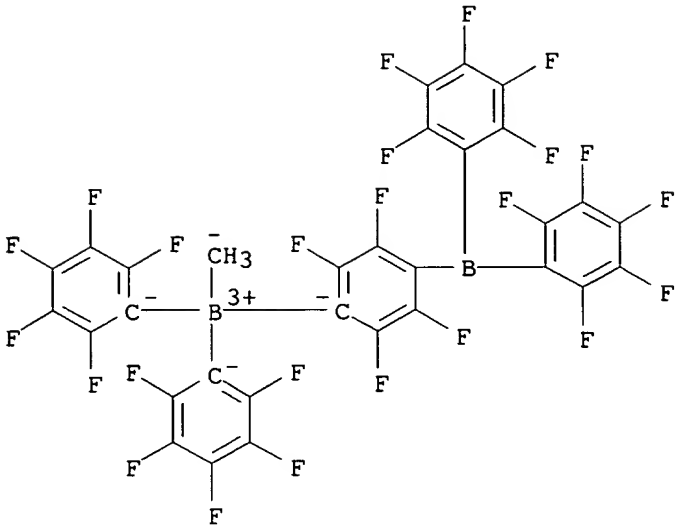
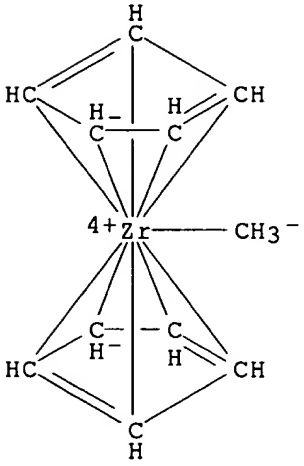
CRN 220503-34-4

CMF C31 H3 B2 F24
CCI CCS



CM 2

CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS



RN 220503-37-7 HCAPLUS
CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, dimethyl[μ-(2,3,5,6-tetrafluoro-1,4-phenylene)]tetrakis(pentafluorophenyl)diborate(2-) (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 220503-36-6

cyclopentadienyl fluorobiphenylborane complex catalyst; metallocene polymn catalyst borane aluminate; constrained geometry catalyst metallocene borane aluminate

IT Polymerization
Polymerization catalysts
(group-transfer; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT Polymerization catalysts
(metallocene; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT Polymer chains
(sequence distribution; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT Molecular dynamics
(solution; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT Polymerization catalysts
(stereospecific; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT Abstraction reaction
Chirality
Crystal structure
Racemization
Reactivity ratio in polymerization
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT **184675-10-3P**
RL: **CAT (Catalyst use)**; PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(**crystal** structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed **polymerization**)

IT 206852-68-8P 206852-74-6P 206852-76-8P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(**crystal** structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 188026-78-0P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(mol. structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 188026-50-8P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(mol. structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 206852-67-7P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(mol. structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 207136-64-9P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(racemic, **crystal** structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 207004-01-1P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(racemic, mol. structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 193149-43-8
RL: CAT (Catalyst use); USES (Uses)
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 184686-71-3P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT **184675-12-5P** 184675-17-0P 184675-19-2P **184686-73-5P**
184686-74-6P 188026-58-6P 188026-61-1P 188026-66-6P 188026-69-9P
188026-72-4P 188026-82-6P **206852-59-7P** 206852-73-5P
207004-00-0P 207004-03-3P 207004-05-5P
207004-06-6P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed **polymerization**)

IT 76-83-5, Trityl chloride 344-04-7, Bromopentafluorobenzene 1093-66-9, 2-Bromononafluorobiphenyl 1109-15-5, Tris(pentafluorophenyl)boron 7446-70-0, Aluminum trichloride, reactions 10294-34-5, Boron trichloride 12636-72-5, Bis(η5-cyclopentadienyl)dimethylzirconium 37206-41-0, Dibenzylbis(η5-cyclopentadienyl)zirconium 67108-80-9, Dimethylbis(η5-pentamethylcyclopentadienyl)zirconium 67506-90-5, Dimethylbis(η5-pentamethylcyclopentadienyl)thorium 81476-64-4, Trimethyl(η5-pentamethylcyclopentadienyl)zirconium 106865-92-3, Bis(η5-1,2-dimethylcyclopentadienyl)dimethylzirconium 113161-86-7, Trimethyl(η5-pentamethylcyclopentadienyl)hafnium 118572-21-7, Dimethylbis[1,3-bis(trimethylsilyl)cyclopentadienyl]zirconium 134366-83-9 135072-62-7 135539-56-9 146814-57-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 193149-50-7P 206852-64-4P 206852-75-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

IT 9002-88-4P 9003-07-0P, Polypropylene 9003-53-6P, Polystyrene

25068-12-6P, Ethylene-styrene copolymer 25085-53-4P, Isotactic polypropylene 25188-97-0P, Syndiotactic poly(methyl methacrylate) 25188-98-1P, Isotactic poly(methyl methacrylate) 25213-02-9P, Ethylene-1-hexene copolymer 206852-61-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed polymerization)

RE.CNT 106 THERE ARE 106 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

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IT **184675-10-3P**
RL: **CAT (Catalyst use)**; PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(**crystal** structure; sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed **polymerization**)

RN 184675-10-3 HCAPLUS

CN Zirconium(1+), tetrakis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]-μ-methyldimethyldi-, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

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CRN 184686-70-2
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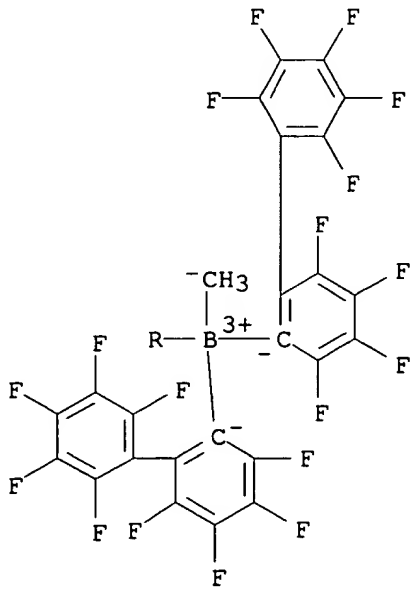
CCI CCS

PAGE 1-A



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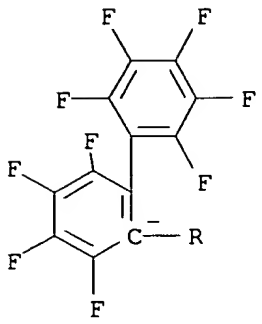

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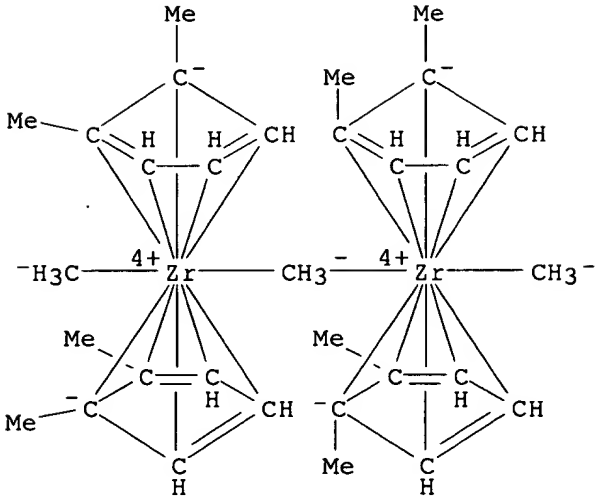


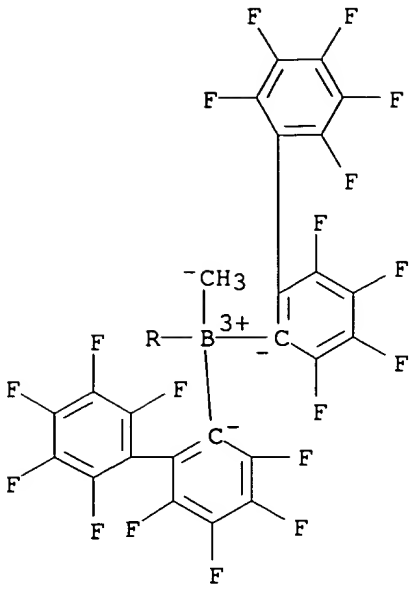
IT **184675-12-5P 184686-73-5P 206852-59-7P**
207004-00-0P 207004-03-3P 207004-05-5P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(sterically encumbered borane and aluminate cocatalysts for tuning cation-anion structure and reactivity in metallocene-catalyzed **polymerization**)

RN 184675-12-5 HCAPLUS
CN Zirconium(1+), μ-methyldimethyltetrakis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

PAGE 1-A



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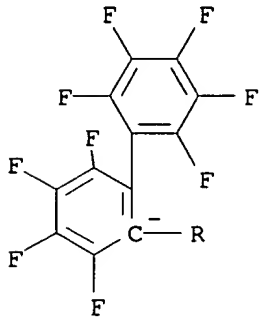

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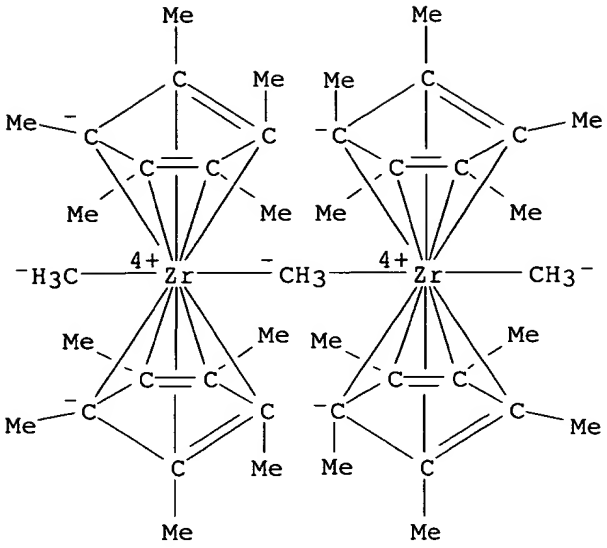
CCI CCS



RN 184686-73-5 HCAPLUS
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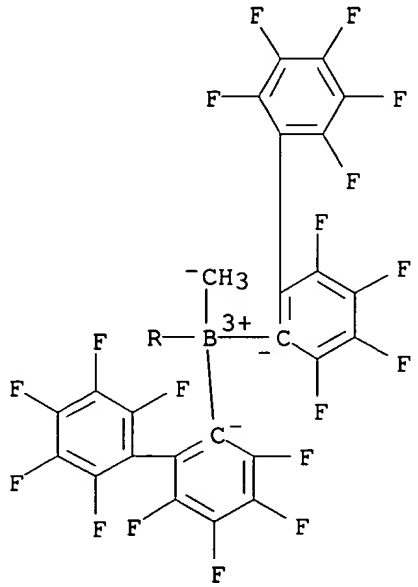
CM 1

CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

PAGE 1-A



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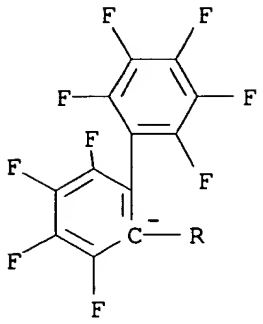

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CRN 174577-52-7
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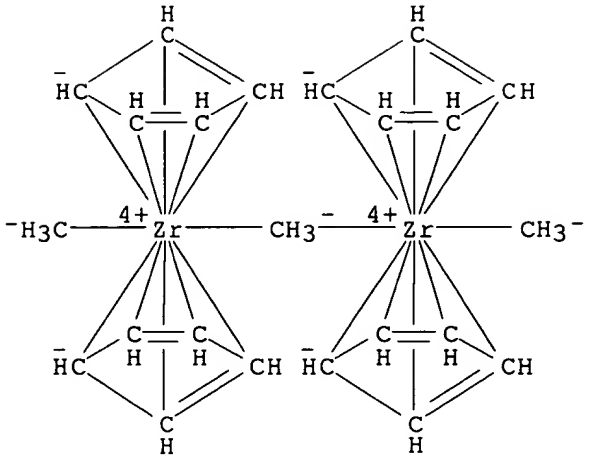
CCI CCS



RN 206852-59-7 HCAPLUS
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CRN 206852-58-6
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CCI CCS

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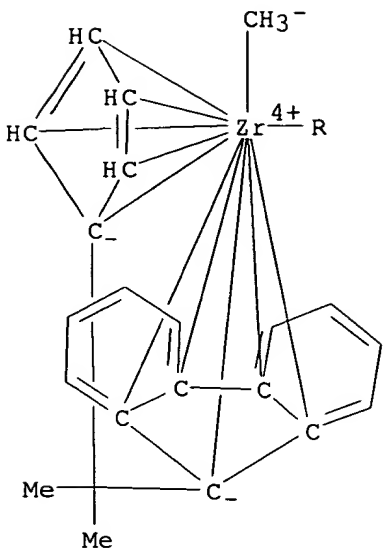

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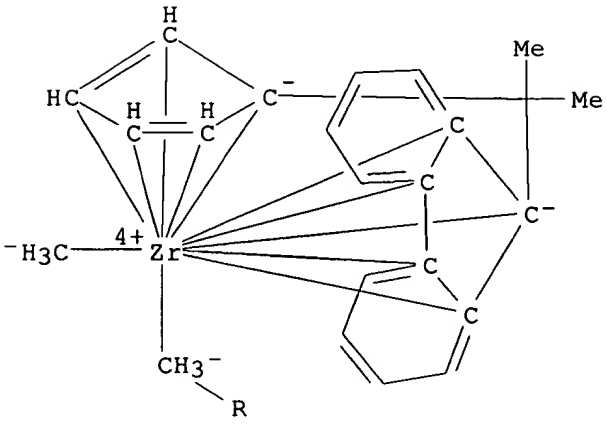

CM 2

CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

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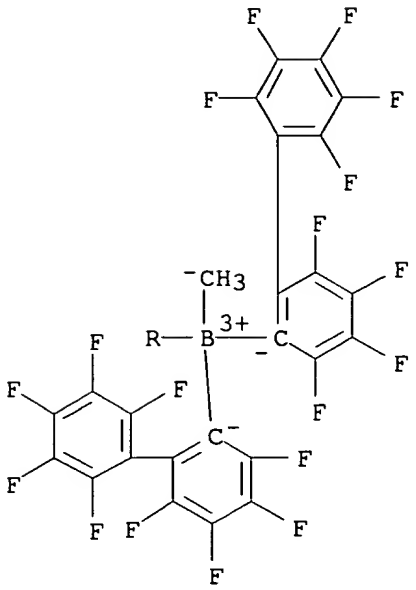

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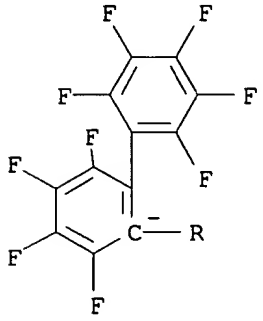

RN 207004-00-0 HCAPLUS
CN Zirconium(1+), bis[(dimethylsilylene)bis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]-μ-methyldimethyldi-, stereoisomer, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

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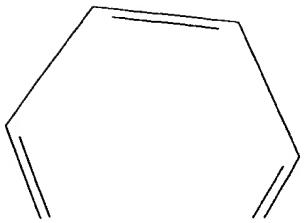
CRN 207003-99-4
CMF C43 H45 Si2 Zr2
CCI CCS

PAGE 1-A



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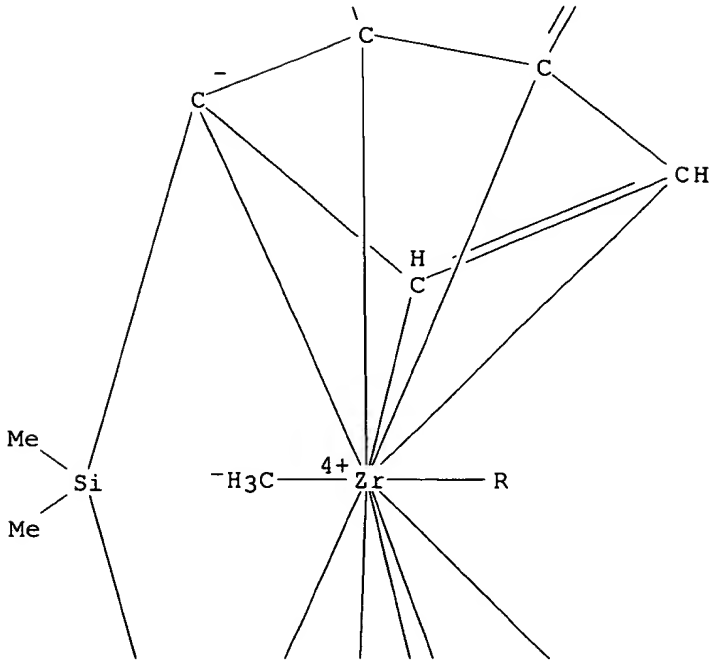

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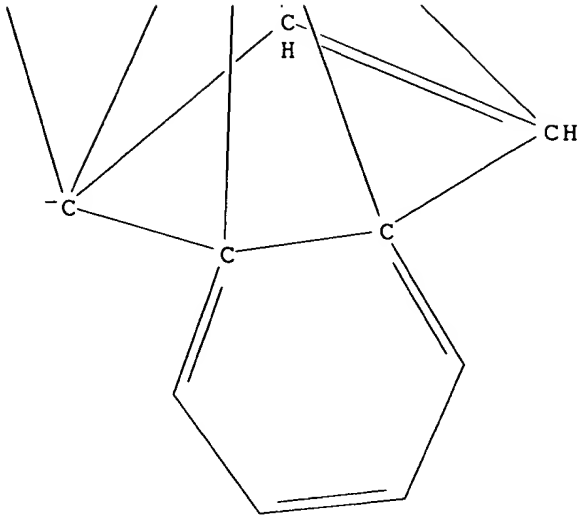

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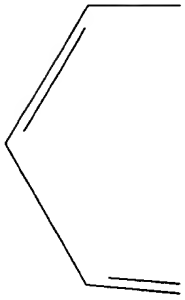
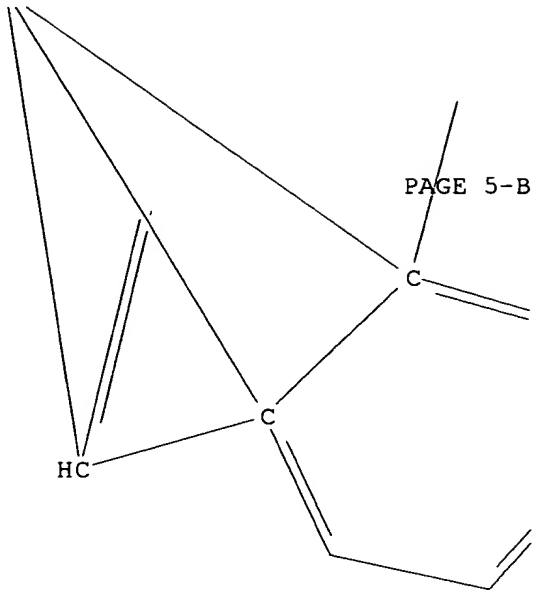


* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *



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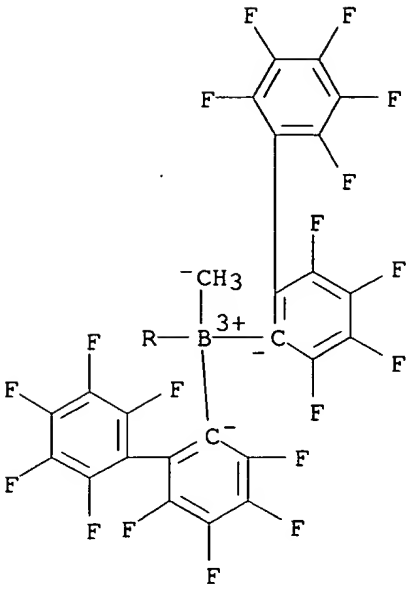
CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

PAGE 1-A



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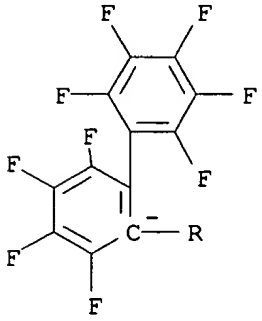

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CN Zirconium(1+), bis[(dimethylsilylene)bis[(1,2,3,3a,7a-η)-1H-inden-1-ylidene]]-μ-methyldimethyldi-, stereoisomer, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

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CCI CCS

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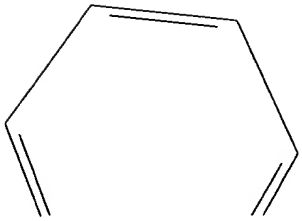

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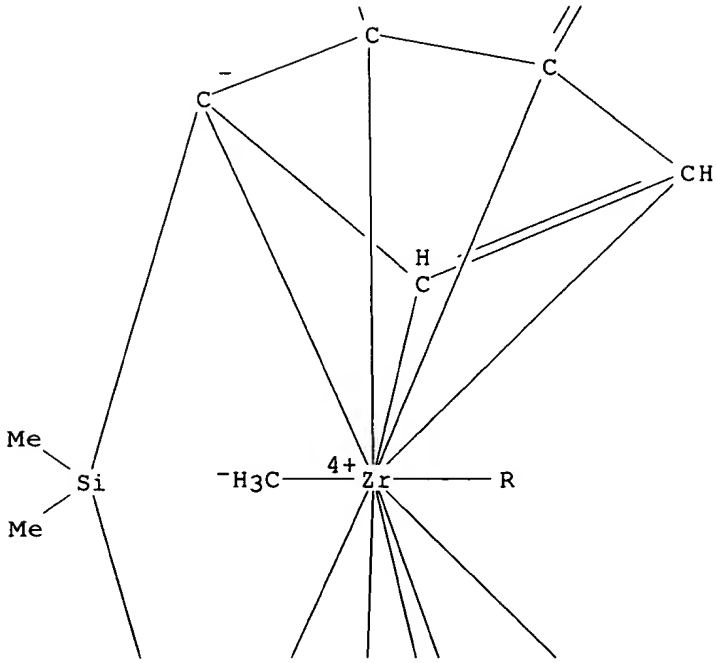

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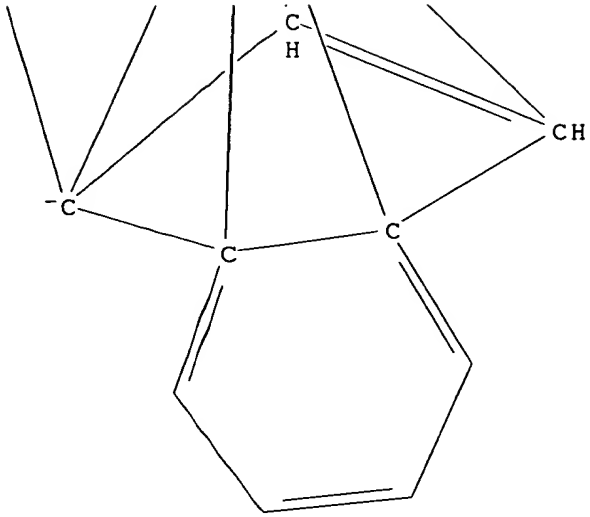

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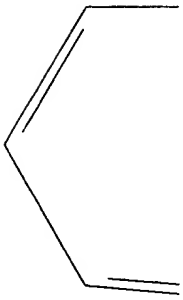

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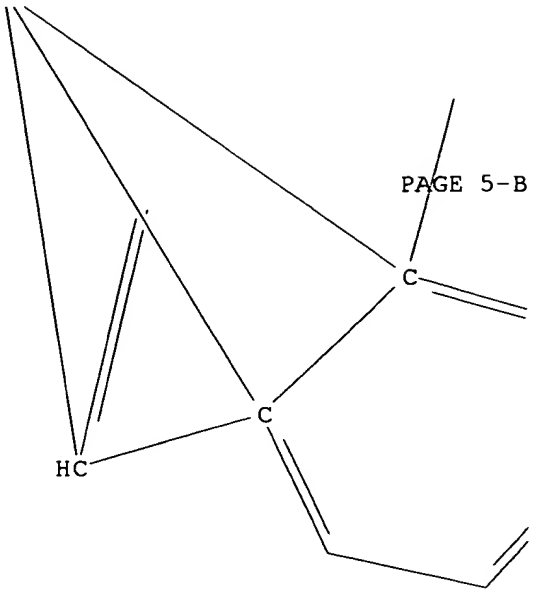

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PAGE 5-C

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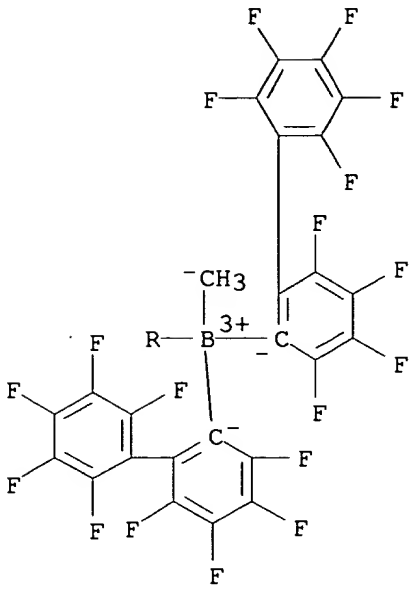
CMF C37 H3 B F27
CCI CCS

PAGE 1-A



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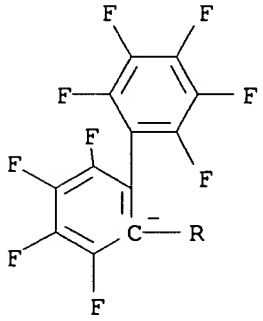

RN 207004-05-5 HCAPLUS
CN Zirconium(1+), bis[η10-2,4-cyclopentadien-1-ylidene(1-methylethylidene)-9H-fluoren-9-ylidene]-μ-methyldimethyldi-, stereoisomer, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

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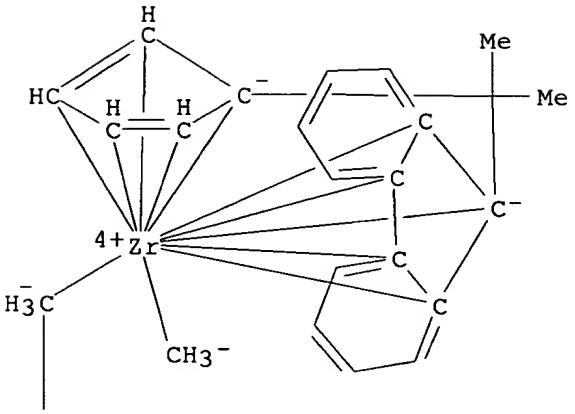
CCI CCS

PAGE 1-A



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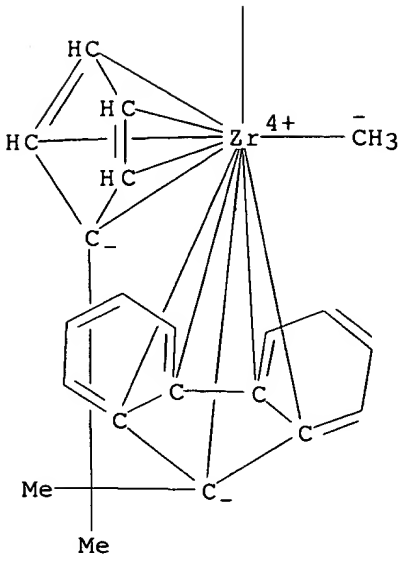

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CCI CCS

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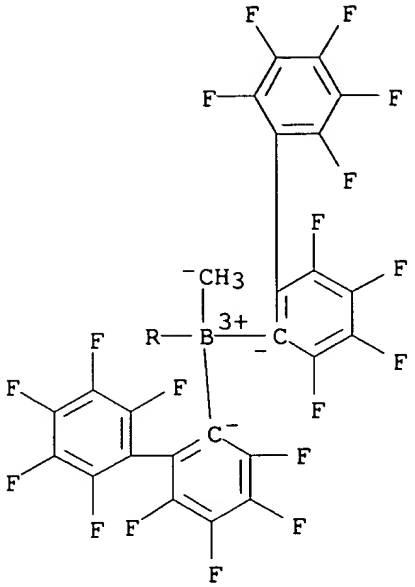

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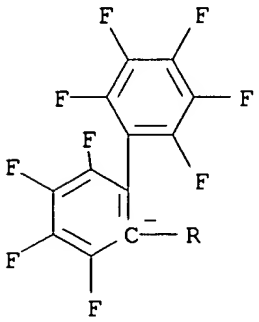


L34 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1998:228800 HCAPLUS
DN 128:321975
ED Entered STN: 23 Apr 1998
TI Reaction of ether and thioether functionalized 1-alkenes with the cationic permethylzirconocene olefin polymerization catalyst [(η5-C5Me5)2ZrMe]+. Molecular structure of the insertion product [(η5-C5Me5)2ZrCH2CH(Me)CH2OEt]+
AU Bijpost, Erik A.; Zuideveld, Martin A.; Meetsma, Auke; Teuben, Jan H.
CS Department of Chemistry, Groningen Centre for Catalytic Olefin Polymerisation, University of Groningen, Groningen, 9747 AG, Neth.
SO Journal of Organometallic Chemistry (1998), 551(1-2), 159-164
CODEN: JORCAI; ISSN: 0022-328X

PB Elsevier Science S.A.
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 75
AB Reaction of [(η5-C5Me5)2ZrMe][MeB(C6F5)3] (I) with (thio)ether-functionalized alkenes: 3-ethoxy-1-propene and 3-(methylthio)-1-propene gives stable insertion products [(η5-C5Me5)2ZrCH2CH(Me)CH2XR][MeB(C6F5)3] (II: X = O, R = Et; III: X = S, R = Me) in which the (thio)ether function is intramolecularly coordinated to zirconium. The mol. structure of II shows a regular 1-oxa-2-zirconacyclopentane in an envelope conformation. The metallacycles in II and III are stable toward further insertion of (functionalized) alkenes and cannot be activated for ethene polymerization by pre-complexation of the (thio)ether function with strong Lewis acids (AlCl3, MgCl2, B(C6F5)3 or [Ph3C]+). The strong alkylating co-catalyst Me3Al regenerates complex I by exchange of the (thio)ether function for Me and thus initiates polymerization of ethene.
ST zirconocene polymn catalyst insertion ethoxypropene methylthiopropene; structure insertion product zirconocene polymn catalyst
IT Polymerization
(mechanism; reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin polymerization catalyst and mol. structure of insertion product)
IT Polymerization catalysts
(metallocene; reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin polymerization catalyst and mol. structure of insertion product)
IT Bond angle
Bond length
Crystal structure
(reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin polymerization catalyst and mol. structure of insertion product)
IT 75-24-1, Trimethylaluminum
RL: CAT (Catalyst use); USES (Uses)
(cocatalyst; reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin polymerization catalyst and mol. structure of insertion product)
IT **133445-52-0**
RL: **CAT (Catalyst use)**; RCT (Reactant); RACT (Reactant or reagent); USES (Uses)
(reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin **polymerization** catalyst and mol. structure of insertion product)
IT 207124-75-2P 207124-77-4P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin polymerization catalyst and mol. structure of insertion product)
IT 557-31-3, 3-Ethoxy-1-propene 10152-76-8, 3-(Methylthio)-1-propene
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin polymerization catalyst and mol. structure of insertion product)
IT **133445-52-0**
RL: **CAT (Catalyst use)**; RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

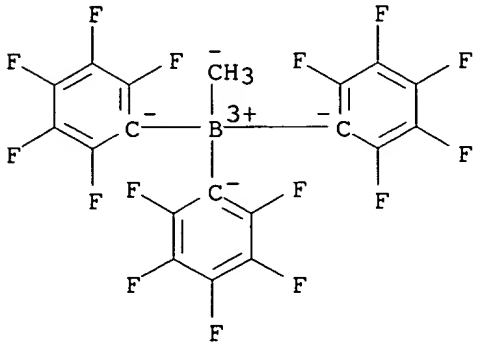
(reaction of ether and thioether functionalized 1-alkenes with cationic permethylzirconocene olefin **polymerization** catalyst and mol. structure of insertion product)

RN 133445-52-0 HCAPLUS

CN Zirconium(1+), methylbis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

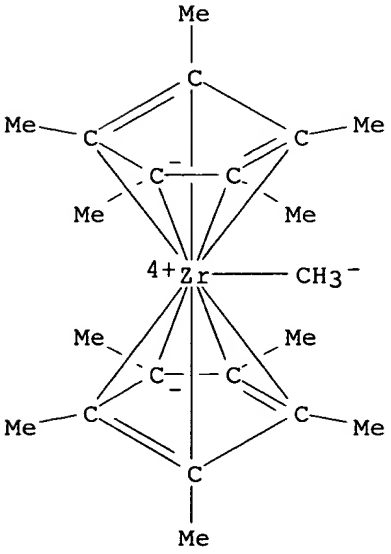
CM 1

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



CM 2

CRN 118611-11-3
CMF C21 H33 Zr
CCI CCS



L34 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:750142 HCAPLUS
DN 127:319318
ED Entered STN: 02 Dec 1997
TI Internal Fluorocarbon Coordination as a Tool for the Protection of Active Catalytic Sites: Experimental Characterization of the Protective Zr···F-C Interaction in the Group 4 Metallocene(butadiene)/B(C6F5)3 Betaine Ziegler Catalyst Systems
AU Karl, Joern; Erker, Gerhard; Froehlich, Roland
CS Organisch-Chemisches Institut, Universitaet Muenster, Muenster, D-48149, Germany
SO Journal of the American Chemical Society (1997), 119(46), 11165-11173
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29
AB The Lewis acid tris(pentafluorophenyl)borane adds to the (butadiene)Group 4 metallocenes (metallocene = Cp2Zr, Cp2Hf, (MeCp)2Zr, (Me3CCp)2Zr) to give the metallocene-(μ-C4H6)-borate-betaine complexes. (Isoprene)zirconocene and (2-phenylbutadiene)zirconocene add the B(C6F5)3 reagent regioselectively at the carbon atom C-4. The complexes all show a pronounced M···F-C interaction with one of the six ortho-B(C6F5)3 fluorine atoms. The resulting metallacyclic structures were characterized by X-ray diffraction of the complexes (Zr···F ≈ 2.40 Å, angle Zr-F-C ≈ 140°). The bridging fluorine atom of the complexes in solution is characterized by an extreme upfield shift of its 19F NMR resonance (δ ≈ -210 to -220 ppm) relative to the signals of the remaining five o-F resonances of the B(C6F5)3 moiety (average δ ≈ -135 ppm). The 19F NMR spectra of the complexes are dynamic even in the noncoordinating solvent toluene-d8. All six o-fluorine signals equilibrate with coalescence temps. around 240 K at 584 MHz to give a single resonance signal at high temperature This fluorine equilibration process of the -B(C6F5)3 end of the metallocene-borate-betaine complexes is very likely to proceed via a rate determining cleavage of the coordinative M···F-C interaction. From the activation barrier of this process, obtained from the dynamic fluorine NMR spectra, Zr···F bond dissociation energies of ca. 8.5 kcal/mol were estimated for the complexes. This magnitude of the M···F-C bond dissociation energy makes the internal fluorocarbon coordination a very suitable tool for protecting active electrophilic metal catalyst centers. The Zr···F-C bond of the complexes is cleaved by the addition of the donor solvent THF with formation of acyclic 1,2-η2-allyl metallocene complexes.
ST metallocene butadiene borate betaine polymn catalyst; Ziegler polymn catalyst metallocene butadiene borate
IT Polymerization catalysts
(Ziegler-Natta; exptl. characterization of protective Zr···F-C interaction in Group 4 metallocene(butadiene)/B(C6F5)3 betaine Ziegler polymerization catalyst systems)
IT Bond angle
Bond length
Crystal structure
(exptl. characterization of protective Zr···F-C

interaction in Group 4 metallocene(butadiene)/B(C6F5)3 betaine Ziegler polymerization catalyst systems)

IT 171003-33-1P 197580-13-5P 197580-16-8P 197580-20-4P 197580-24-8P 197580-29-3P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(exptl. characterization of protective Zr···F-C interaction in Group 4 metallocene(butadiene)/B(C6F5)3 betaine Ziegler polymerization catalyst systems)

IT **197580-12-4P 197580-14-6P 197580-18-0P 197580-22-6P 197580-26-0P 197580-32-8P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(exptl. characterization of protective Zr···F-C interaction in Group 4 metallocene(butadiene)/B(C6F5)3 betaine Ziegler **polymerization** catalyst systems)

IT 1109-15-5, Tris(pentafluorophenyl)boron 75361-73-8 75374-50-4 80185-89-3 101518-70-1 113667-86-0 197580-35-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; exptl. characterization of protective Zr···F-C interaction in Group 4 metallocene(butadiene)/B(C6F5)3 betaine Ziegler polymerization catalyst systems)

IT **197580-12-4P 197580-14-6P 197580-18-0P 197580-22-6P 197580-26-0P 197580-32-8P**
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(exptl. characterization of protective Zr···F-C interaction in Group 4 metallocene(butadiene)/B(C6F5)3 betaine Ziegler **polymerization** catalyst systems)

RN 197580-12-4 HCAPLUS

CN Zirconium, [μ-[(1-η:2,3,4-η)-2-butene-1,4-diyl]]bis(η5-2,4-cyclopentadien-1-yl)(tetrahydrofuran)[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

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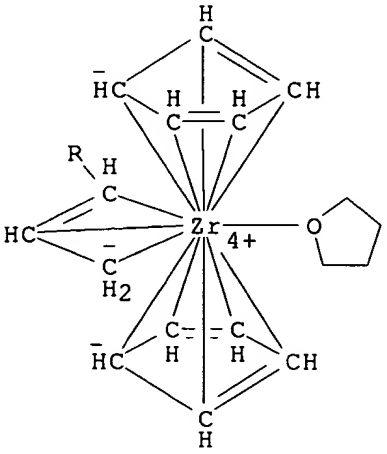

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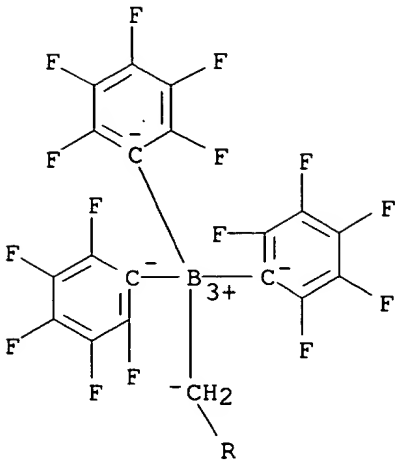

RN 197580-14-6 HCAPLUS
CN Hafnium, [μ-[(1-η:2,3,4-η)-2-butene-1,4-diyl]]bis(η5-2,4-cyclopentadien-1-yl)(tetrahydrofuran)[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

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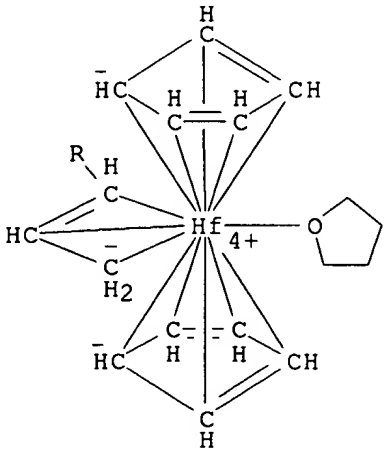

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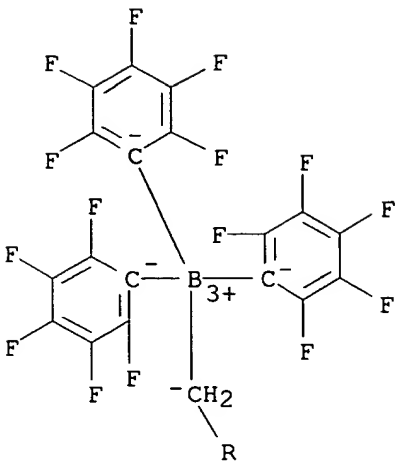

RN 197580-18-0 HCAPLUS
CN Zirconium, [μ-[(1-η:2,3,4-η)-2-butene-1,4-diyl]]bis[(1,2,3,4,5-η)-1-methyl-2,4-cyclopentadien-1-yl](tetrahydrofuran)[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

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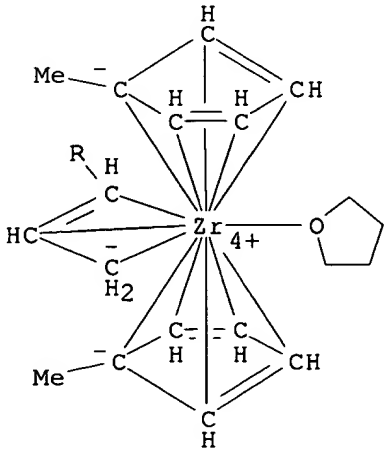

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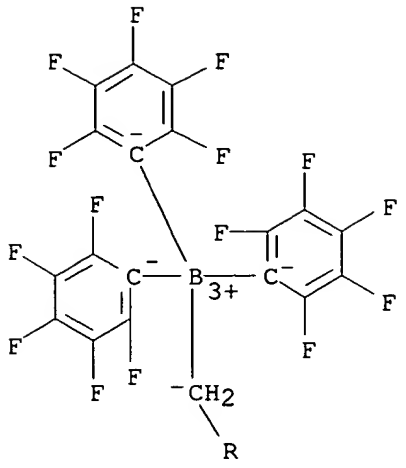
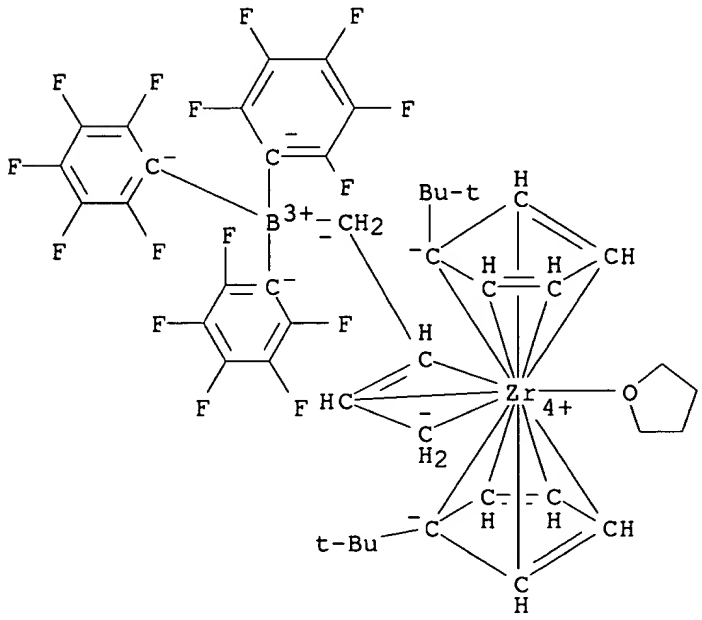


RN 197580-22-6 HCAPLUS
CN Zirconium, [μ-[(1-η:2,3,4-η)-2-butene-1,4-diyl]]bis[(1,2,3,4,5-η)-1-(1,1-dimethylethyl)-2,4-cyclopentadien-1-yl](tetrahydrofuran)[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)



RN 197580-26-0 HCAPLUS
CN Zirconium, bis(η5-2,4-cyclopentadien-1-yl)[μ-[(1,2,3-η:4-η)-2-methyl-2-butene-1,4-diyl]](tetrahydrofuran)[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

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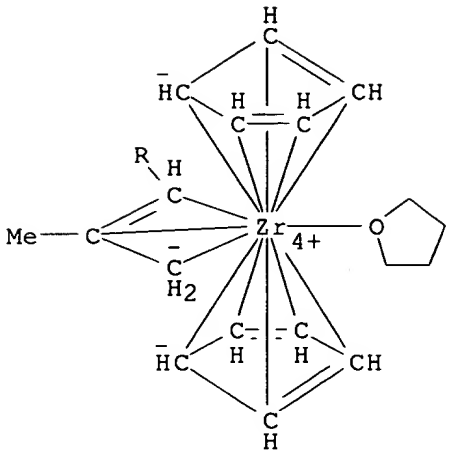

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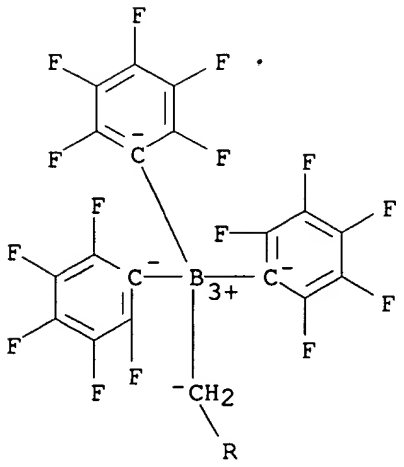

RN 197580-32-8 HCAPLUS
CN Zirconium, bis(η5-2,4-cyclopentadien-1-yl)[μ-[(1,2,3-η:4-η)-2-phenyl-2-butene-1,4-diyl]](tetrahydrofuran)[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

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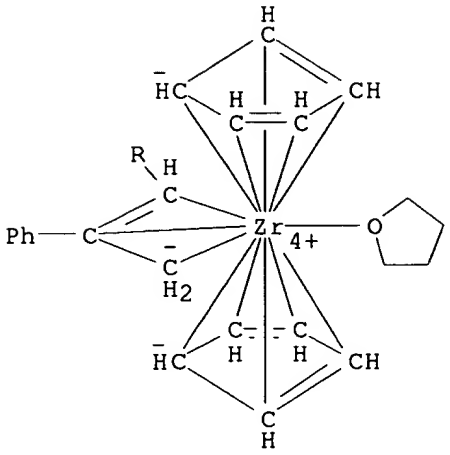

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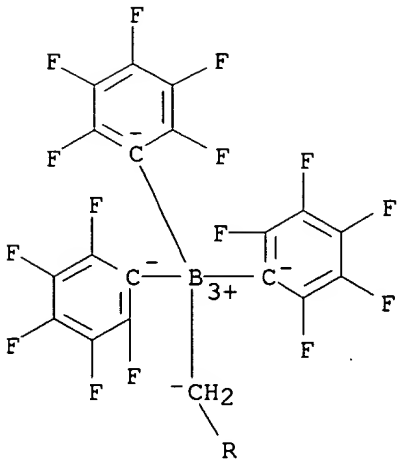

L34 ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:324328 HCAPLUS
DN 127:5389
ED Entered STN: 22 May 1997
TI Intramolecular Ion-Ion Interactions in Zwitterionic Metallocene Olefin Polymerization Catalysts Derived from "Tucked-In" Catalyst Precursors and the Highly Electrophilic Boranes XB(C6F5)2 (X = H, C6F5)
AU Sun, Yimin; Spence, Rupert E. v. H.; Piers, Warren E.; Parvez, Masood; Yap, Glenn P. A.
CS Department of Chemistry, University of Calgary, Calgary, AB, T2N 1N4, Can.
SO Journal of the American Chemical Society (1997), 119(22), 5132-5143
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal

LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 75
AB The reactions of so called "tuck-in" permethyl zirconocene compds. Cp*(η5-η1-C5Me4CH2)ZrX (X = Cl (1a), C6H5 (1b), CH3 (1c)) with the highly electrophilic boranes HB(C6F5)2 and B(C6F5)3 are described. The products are zwitterionic olefin polymerization catalysts. Reactions with 1a and 1b yielded single products cleanly, but reactions with tuck-in Me starting material 1c gave mixts. Spectroscopic and structural studies showed that the electrophilic zirconium center in the product zwitterions was stabilized by a variety of mechanisms. In the products of reaction between 1a and 1b with HB(C6F5)2, Cp*[η5,η1-C5Me4CH2B(C6F5)2(μ-H)]ZrX (X = Cl (2a), 74%, C6H5 (2b, 62%)), the metal is chelated by a pendant hydridoborate moiety. Chloride product 2a was characterized **crystallog**. In the reaction of B(C6F5)3 with 1a, the fluxional zwitterionic product Cp*[η5-C5Me4CH2B(C6F5)3]ZrCl (3a, 84%) is stabilized by a weak donor interaction between one of the ortho fluorine atoms of the -CH2B-(C6F5)3 counterion and the zirconium center (Zr-F = 2.267(5) Å). In the product of the reaction between 1b and B(C6F5)3, Cp*[η5-C5Me4CH2B(C6F5)3]ZrC6H5 (3b, 82%), a similar ortho-fluorine interaction was found in a yellow kinetic product (y-3b), which converted upon heating gently to a thermodn. orange polymorph (o-3b) in which the zirconium center is compensated via an agostic interaction from an ortho C-H bond of the Ph group and an interaction between the methylene group of the -CH2B-(C6F5)3 counteranion. These compds. were both characterized by X-ray **crystallog**. Zwitterion o-3b reacts with H2 to form the zwitterionic hydride Cp*[η5-C5Me4CH2B(C6F5)3]ZrH (4, 77%), characterized by NMR spectroscopy and X-ray **crystallog**. to reveal a return to the ortho-fluorine mode of stabilization. Compds. 2a, 3a, o-3b, and 4 were all found to be active ethylene polymerization catalysts; the chloride derivs. required minimal amts. of methylaluminoxane (MAO) to alkylate the zirconium center. Polymerization data are discussed in light of the structural findings for the catalysts employed.
ST zwitterionic zirconocene borane catalyst prepn; **crystal** structure zwitterionic zirconocene borane complex; ethylene polymn zwitterionic zirconocene borane catalyst; polyethylene synthesis zwitterionic zirconocene borane catalyst
IT Aluminoxanes
RL: CAT (Catalyst use); USES (Uses)
(Me, activator; intramol. ion-ion interactions in zwitterionic zirconocene olefin polymerization catalysts derived from "tucked-in" precursors and perfluorophenylboranes)
IT Bond angle
Bond length
Crystal structure
NMR (nuclear magnetic resonance)
(intramol. ion-ion interactions in zwitterionic zirconocene olefin polymerization catalysts derived from "tucked-in" precursors and perfluorophenylboranes)
IT Polymerization catalysts
(zwitterionic; intramol. ion-ion interactions in zwitterionic zirconocene olefin polymerization catalysts derived from "tucked-in" precursors and perfluorophenylboranes)
IT 1109-15-5, Tris(pentafluorophenyl)borane 105501-02-8 135525-04-1 165612-94-2, Bis(pentafluorophenyl)borane 190327-20-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(catalyst preparation; intramol. ion-ion interactions in zwitterionic zirconocene olefin polymerization catalysts derived from "tucked-in" precursors and perfluorophenylboranes)

IT 190327-21-0P 190327-22-1P 190327-23-2P **190327-24-3P** **190327-25-4P**
RL: **CAT (Catalyst use)**; PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(intramol. ion-ion interactions in zwitterionic zirconocene olefin **polymerization** catalysts derived from "tucked-in" precursors and perfluorophenylboranes)

IT 9002-88-4P, Polyethylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(intramol. ion-ion interactions in zwitterionic zirconocene olefin polymerization catalysts derived from "tucked-in" precursors and perfluorophenylboranes)

IT **190327-24-3P** **190327-25-4P**
RL: **CAT (Catalyst use)**; PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(intramol. ion-ion interactions in zwitterionic zirconocene olefin **polymerization** catalysts derived from "tucked-in" precursors and perfluorophenylboranes)

RN 190327-24-3 HCAPLUS

CN Zirconium, [μ-[η:η5-methylene(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)]][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]phenyl[tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

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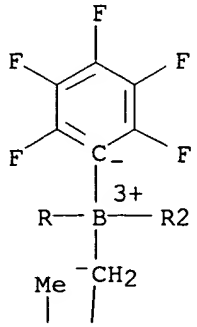

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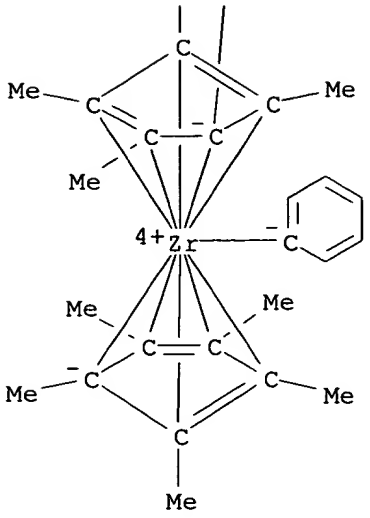

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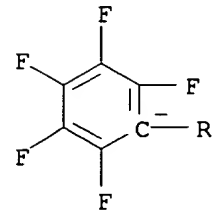

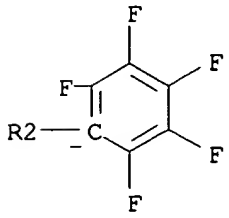

RN 190327-25-4 HCAPLUS
CN Zirconium, hydro[μ-[η:η5-methylene(2,3,4,5-tetramethyl-2,4-cyclopentadien-1-ylidene)]][(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl][tris(pentafluorophenyl)boron]- (9CI) (CA INDEX NAME)

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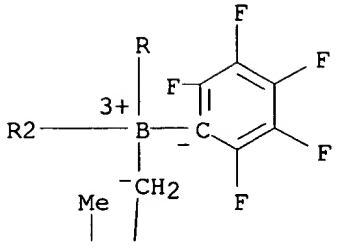

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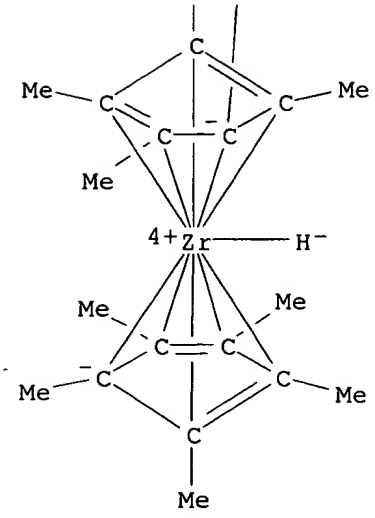

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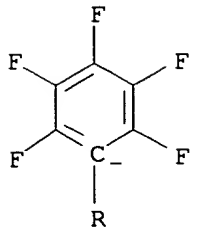
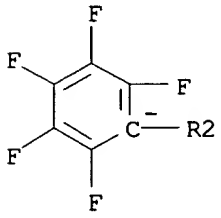




L34 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:127122 HCAPLUS
DN 126:118033
ED Entered STN: 25 Feb 1997
TI Cationic Metallocene Polymerization Catalysts Based on Tetrakis(pentafluorophenyl)borate and Its Derivatives. Probing the Limits of Anion "Noncoordination" via a Synthetic, Solution Dynamic, Structural, and Catalytic Olefin Polymerization Study
AU Jia, Li; Yang, Xinmin; Stern, Charlotte L.; Marks, Tobin J.
CS Department of Chemistry, Northwestern University, Evanston, IL, 60208-3113, USA
SO Organometallics (1997), 16(5), 842-857
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal
LA English
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 22, 35, 75
AB The synthesis and properties of two soluble, weakly coordinating derivs. of the tetrakis(perfluoroaryl)borate anion B(4-C6F4TBS)4- and B(4-C6F4TIPS)4- (TBS = tert-butyldimethylsilyl and TIPS = triisopropylsilyl) are reported. Reaction of the trityl salts of the above anions with a variety of Zr and Th L2MMe2 complexes in benzene or toluene affords the cationic ion-paired Me complexes L2MMe+X- or the corresponding hydrido complexes L2MH+X- (L2 = bis(cyclopentadienyl)- or cyclopentadienylamido-type ligand) when the reaction is carried out under dihydrogen. The solid state structure of (Me5Cp)2ThMe+B(C6F5)4- was characterized by x-ray diffraction. The B(C6F5)4--based zirconocenium Me complexes L2MMe+ are unstable at room temperature with respect to, among other factors, intramol. C-H activation of the ligand framework. In general, the thermal stabilities of the B(C6F4TBS)4-- and B(C6F4TIPS)4--derived complexes are greater than those of the corresponding B(C6F5)4-- and MeB(C6F5)3--derived analogs. The relative coordinative tendencies of MeB(C6F5)3-, B(C6F5)4-, B(C6F4TBS)4-, and B(C6F4TIPS)4- are estimated from the solution spectroscopic information and the structural dynamics of the ion-pairs and follow the order MeB(C6F5)3-

> B(C6F4TBS)4- ≈ B(C6F4TIPS)4- > B(C6F5)4-. The coordination of the neutral metallocene precursors to the cationic metallocenes is found to compete with counteranion coordination. Arene solvent coordination to the Zr constrained geometry cation [(Me4Cp)SiMe2(NtBu)]ZrMe+ is also observed when B(C6F5)4- is the counteranion. (1,2-Me2Cp)2ZrMe+B(C6F4TBS)4- undergoes slow decomposition under an inert atmospheric to afford [(1,2-Me2Cp)2ZrF]2(μ-F)+B(C6F4TBS)4-, which was characterized by x-ray diffraction. The olefin polymerization activity and thermal stability of the zirconocene catalysts reaches a maximum when B(C6F4TBS)4- and B(C6F4TIPS)4- are used as counteranions. The polymerization activity of the Zr constrained geometry complex also reaches a maximum in aromatic solvents when B(C6F5)4- is used as the counteranion, apparently due to solvent coordination.

ST **crystal** structure thorium zirconium cyclopentadienyl tetraarylborate; mol structure thorium zirconium cyclopentadienyl tetraarylborate; polymn catalyst thorium zirconium cyclopentadienyl tetraarylborate; metallocene tetraarylborate olefin polymn catalyst; zirconocenium tetraarylborate prepn structure polymn catalysis; thorocenium tetraarylborate prepn structure polymn catalysis; coordination tetraarylborate thorium zirconium; ion pair dissocn kinetics metallocene tetraarylborate; thorium cyclopentadienyl tetraarylborate prepn structure catalysis; zirconium cyclopentadienyl tetraarylborate prepn structure catalysis

IT Dissociation kinetics
(ion-pair; of metallocene cations and arylborate anions)

IT Complexation
(of metallocene cations with arylborate anions, neutral metal alkyls and solvent mols.)

IT **Crystal** structure
Molecular structure
(of thorium and zirconium cyclopentadienyl complex tetraarylborates)

IT Ion pairs
(of thorium and zirconium cyclopentadienyl complexes with tetraarylborates and related anions)

IT Polymerization catalysts
(thorium and zirconium cyclopentadienyl complex tetraarylborates for olefins)

IT Polyolefins
RL: SPN (Synthetic preparation); PREP (Preparation)
(thorium and zirconium cyclopentadienyl tetraarylborates as catalysts for preparation of)

IT Metallocenes
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(thorocenes; preparation, **crystal** structure, solution dynamic behavior and stability and catalytic activity for olefin polymerization of tetraarylborate ion-paired cationic)

IT Metallocenes
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(zirconocenes; preparation, **crystal** structure, solution dynamic behavior and stability and catalytic activity for olefin polymerization of tetraarylborate ion-paired cationic)

IT 173687-49-5 **174577-43-6**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) tetrakis(pentafluorophenyl)borate(1-)
RL: **CAT (Catalyst use)**; USES (Uses)

(ethylene **polymerization** in presence of)

IT 76-83-5, Triphenylmethyl chloride 1559-88-2, 1-Bromo-2,3,5,6-tetrafluorobenzene 10294-34-5, Trichloroborane 12636-72-5, Bis(η5-cyclopentadienyl)dimethylzirconium 67108-80-9, Dimethylbis(η5-pentamethylcyclopentadienyl)zirconium 67506-90-5, Dimethylbis(η5-pentamethylcyclopentadienyl)thorium 69739-34-0, tert-Butyldimethylsilyl trifluoromethanesulfonate 80522-42-5, Triisopropylsilyl trifluoromethanesulfonate 106865-92-3, Bis(η5-1,2-dimethylcyclopentadienyl)dimethylzirconium 135539-56-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of tetraarylborates of thorium and zirconium cyclopentadienyl complexes)

IT 136040-19-2P, Triphenylmethylium tetrakis(pentafluorophenyl)borate(1-) 167172-21-6P, tert-Butyldimethyl(2,3,5,6-tetrafluorophenyl)silane 167172-22-7P, Triisopropyl(2,3,5,6-tetrafluorophenyl)silane 167172-26-1P, Triphenylmethylium tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate 167172-28-3P, Triphenylmethylium tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate 172318-95-5P 185855-33-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(for preparation of tetraarylborates of thorium and zirconium cyclopentadienyl complexes)

IT 185855-50-9
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); FORM (Formation, nonpreparative); PROC (Process)
(formation and dynamic behavior in toluene)

IT 185855-51-0P, (4-(tert-Butyldimethylsilyl)tetrafluorophenyl)bis(η5-cyclopentadienyl)(methyl)zirconium
RL: SPN (Synthetic preparation); PREP (Preparation)
(formation in thermolysis of zirconium cyclopentadienyl Me tetraarylborate in benzene)

IT 132884-30-1P 185855-44-1P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and **crystal** structure of)

IT 132884-34-5P, (μ-Methyl)bis(methylbis(η5-pentamethylcyclopentadienyl)thorium)(1+) tetrakis(pentafluorophenyl)borate(1-) 185855-42-9P, (μ-Methyl)bis(bis(η5-1,2-dimethylcyclopentadienyl)(methyl)zirconium)(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-)
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and equilibrium constant for formation of)

IT 185855-46-3P, Bis(η5-pentamethylcyclopentadienyl)(η3-2-propenyl)thorium(1+) tetrakis(pentafluorophenyl)borate(1-) 185855-48-5P, Bis(η5-1,2-dimethylcyclopentadienyl)(methyl)(tetrahydrofuran)zirconium (1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-)
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **167172-31-8P**, Bis(η5-1,2-dimethylcyclopentadienyl)(methyl)zirconium(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-) **167172-32-9P**, Bis(η5-1,2-dimethylcyclopentadienyl)(methyl)zirconium(1+) tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate(1-) 185855-39-4P
RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(preparation, **crystal** structure, solution dynamic behavior stability

and catalytic activity for olefin **polymerization** of thorium and zirconium cyclopentadienyl arylborates)

IT 132884-29-8P, Methylbis(η5-pentamethylcyclopentadienyl)thorium(1+) tetrakis(pentafluorophenyl)borate(1-) **167172-29-4P**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-) **167172-30-7P**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate(1-) **167172-33-0P**, Hydrobis(η5-pentamethylcyclopentadienyl)zirconium(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-) **167172-34-1P**, Hydrobis(η5-pentamethylcyclopentadienyl)zirconium(1+) tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate(1-) **185855-35-0P**, Bis(η5-1,2-dimethylcyclopentadienyl)(hydro)zirconium(1+) tetrakis(pentafluorophenyl)borate(1-) **185855-36-1P**, Hydrobis(η5-pentamethylcyclopentadienyl)zirconium(1+) tetrakis(pentafluorophenyl)borate(1-) 185855-37-2P 185855-38-3P 185855-40-7P, Methylbis(η5-pentamethylcyclopentadienyl)thorium(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-) 185855-41-8P, Methylbis(η5-pentamethylcyclopentadienyl)thorium(1+) tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate(1-)
RL: **CAT (Catalyst use)**; PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, **crystal** structure, solution dynamic behavior stability and catalytic activity for olefin **polymerization** of thorium and zirconium cyclopentadienyl arylborates)

IT **133445-49-5**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) methyltris(pentafluorophenyl)borate(1-) **133445-51-9**, Bis(η5-1,2-dimethylcyclopentadienyl)(methyl)zirconium(1+) methyltris(pentafluorophenyl)borate(1-) **133445-52-0**, Methylbis(η5-pentamethylcyclopentadienyl)zirconium(1+) methyltris(pentafluorophenyl)borate(1-)
RL: **CAT (Catalyst use)**; USES (Uses)
(propylene **polymerization** in presence of)

IT 74-85-1, Ethene, reactions 115-07-1, 1-Propene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(thorium and zirconium cyclopentadienyl tetraarylborates as catalysts for polymerization of)

IT 9002-88-4P, Polyethylene 9003-07-0P, Polypropylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(thorium and zirconium cyclopentadienyl tetraarylborates as catalysts for preparation of)

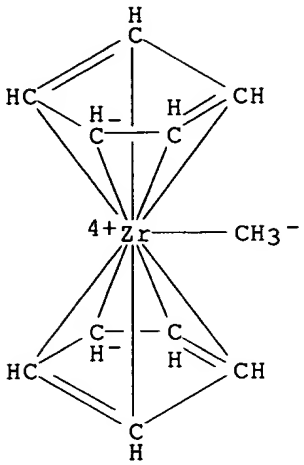
IT **174577-43-6**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) tetrakis(pentafluorophenyl)borate(1-)
RL: **CAT (Catalyst use)**; USES (Uses)
(ethylene **polymerization** in presence of)

RN 174577-43-6 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

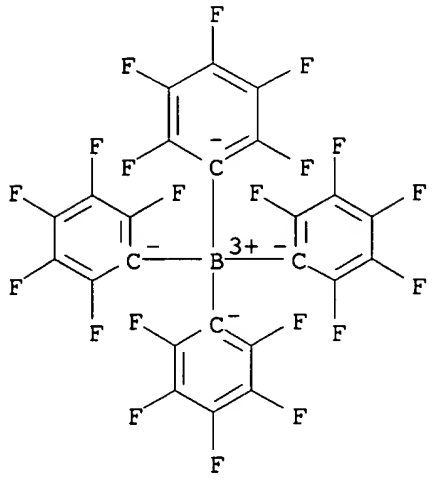
CM 1

CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS



CM 2

CRN 47855-94-7
CMF C24 B F20
CCI CCS

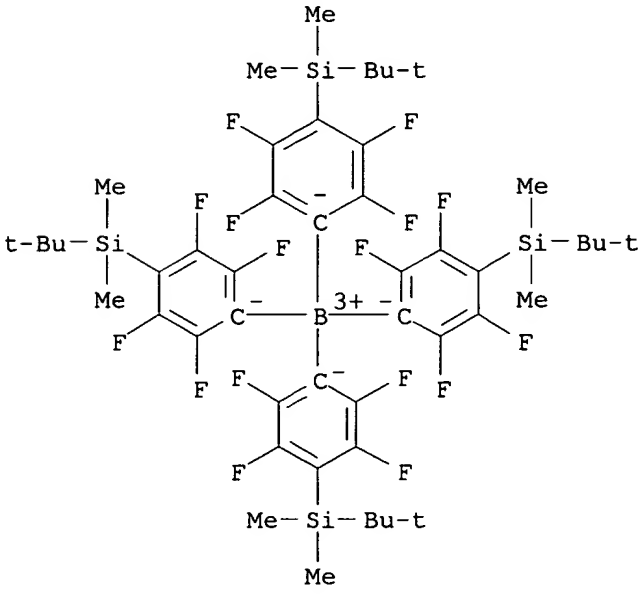


IT **167172-31-8P**, Bis(η5-1,2-dimethylcyclopentadienyl)(methyl)zirconium(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-)
167172-32-9P, Bis(η5-1,2-dimethylcyclopentadienyl)(methyl)zirconium(1+) tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate(1-)
RL: **CAT (Catalyst use)**; PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(preparation, **crystal** structure, solution dynamic behavior stability and catalytic activity for olefin **polymerization** of thorium and zirconium cyclopentadienyl arylborates)
RN 167172-31-8 HCAPLUS

CN Zirconium(1+), bis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]methyl-, tetrakis[4-[(1,1-dimethylethyl)dimethylsilyl]-2,3,5,6-tetrafluorophenyl]borate(1-) (9CI) (CA INDEX NAME)

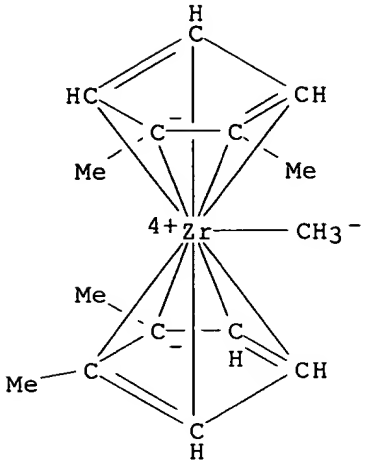
CM 1

CRN 167172-25-0
CMF C48 H60 B F16 Si4
CCI CCS



CM 2

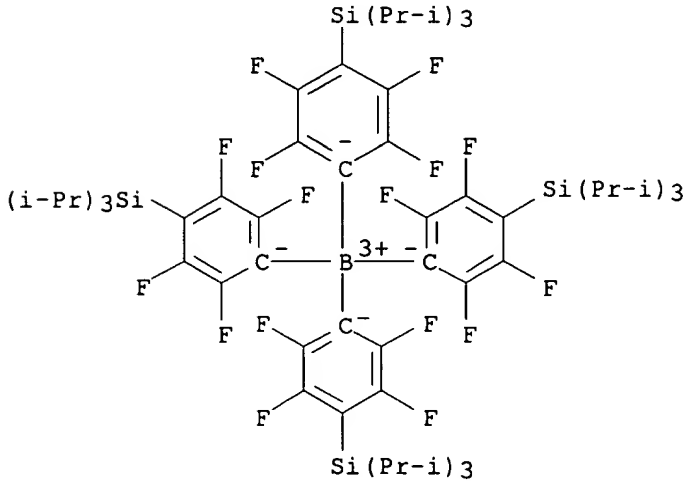
CRN 133445-50-8
CMF C15 H21 Zr
CCI CCS



RN 167172-32-9 HCAPLUS
CN Zirconium(1+), bis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]methyl-, tetrakis[2,3,5,6-tetrafluoro-4-[tris(1-methylethyl)silyl]phenyl]borate(1-) (9CI) (CA INDEX NAME)

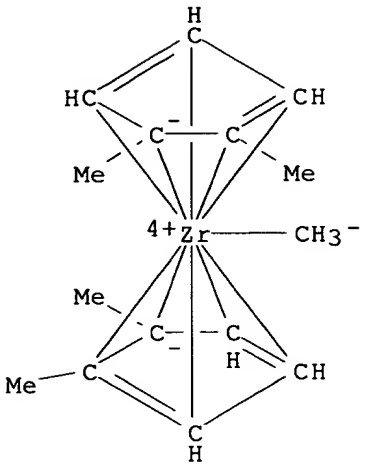
CM 1

CRN 167172-27-2
CMF C60 H84 B F16 Si4
CCI CCS



CM 2

CRN 133445-50-8
CMF C15 H21 Zr
CCI CCS



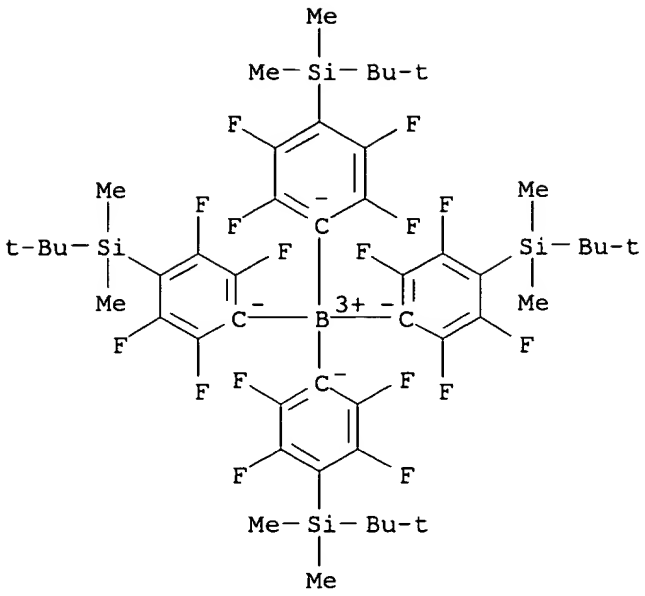
IT **167172-29-4P**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-) **167172-30-7P**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate(1-) **167172-33-0P**, Hydrobis(η5-pentamethylcyclopentadienyl)zirconium(1+) tetrakis(4-(tert-butyldimethylsilyl)tetrafluorophenyl)borate(1-) **167172-34-1P**, Hydrobis(η5-pentamethylcyclopentadienyl)zirconium(1+) tetrakis(tetrafluoro-4-(triisopropylsilyl)phenyl)borate(1-) **185855-35-0P**, Bis(η5-1,2-dimethylcyclopentadienyl)(hydro)zirconium(1+) tetrakis(pentafluorophenyl)borate(1-) **185855-36-1P**, Hydrobis(η5-pentamethylcyclopentadienyl)zirconium(1+) tetrakis(pentafluorophenyl)borate(1-)
RL: **CAT (Catalyst use)**; PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation, **crystal** structure, solution dynamic behavior stability and catalytic activity for olefin **polymerization** of thorium and zirconium cyclopentadienyl arylborates)

RN 167172-29-4 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, tetrakis[4-[(1,1-dimethylethyl)dimethylsilyl]-2,3,5,6-tetrafluorophenyl]borate(1-) (9CI) (CA INDEX NAME)

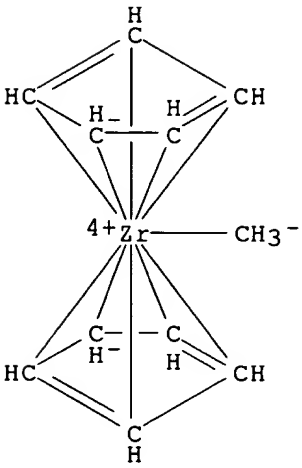
CM 1

CRN 167172-25-0
CMF C48 H60 B F16 Si4
CCI CCS



CM 2

CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS

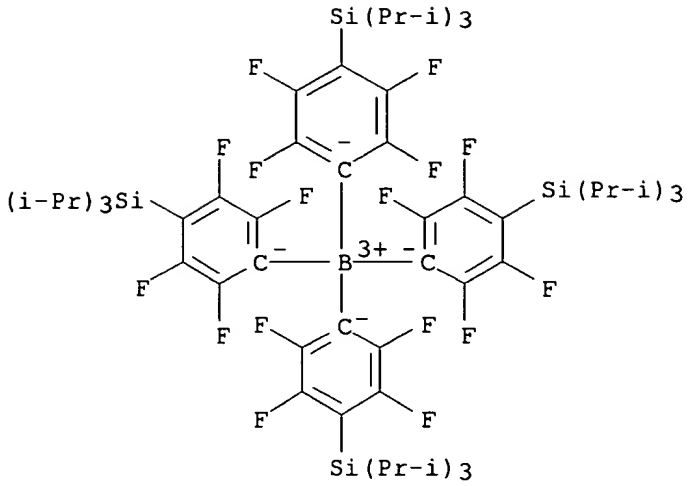


RN 167172-30-7 HCAPLUS
CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, tetrakis[2,3,5,6-tetrafluoro-4-[tris(1-methylethyl)silyl]phenyl]borate(1-) (9CI) (CA INDEX NAME)

CM 1

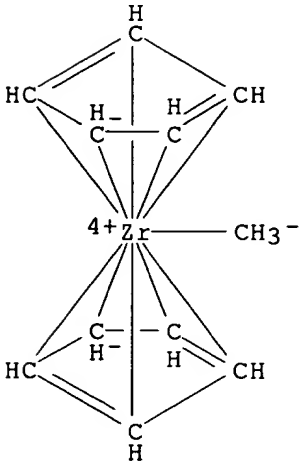
CRN 167172-27-2

CMF C60 H84 B F16 Si4
CCI CCS



CM 2

CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS

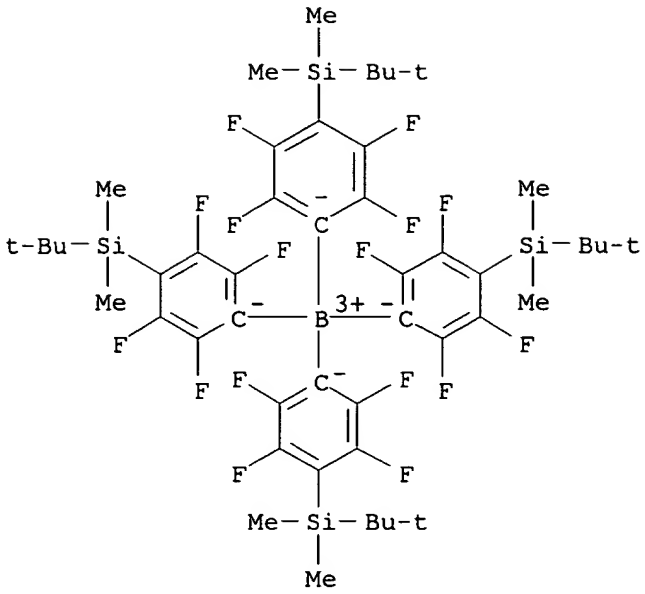


RN 167172-33-0 HCAPLUS
CN Zirconium(1+), hydrobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, tetrakis[4-[(1,1-dimethylethyl)dimethylsilyl]-2,3,5,6-tetrafluorophenyl]borate(1-) (9CI) (CA INDEX NAME)

CM 1

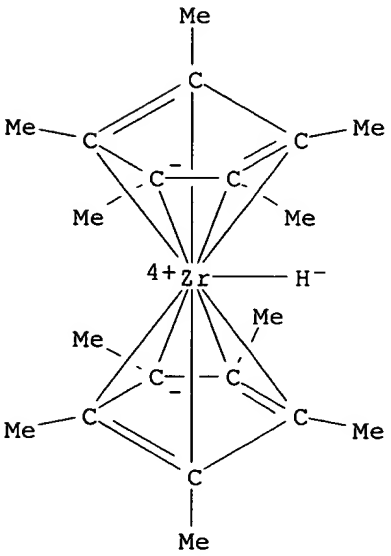
CRN 167172-25-0
CMF C48 H60 B F16 Si4

CCI CCS



CM 2

CRN 143565-16-6
CMF C20 H31 Zr
CCI CCS

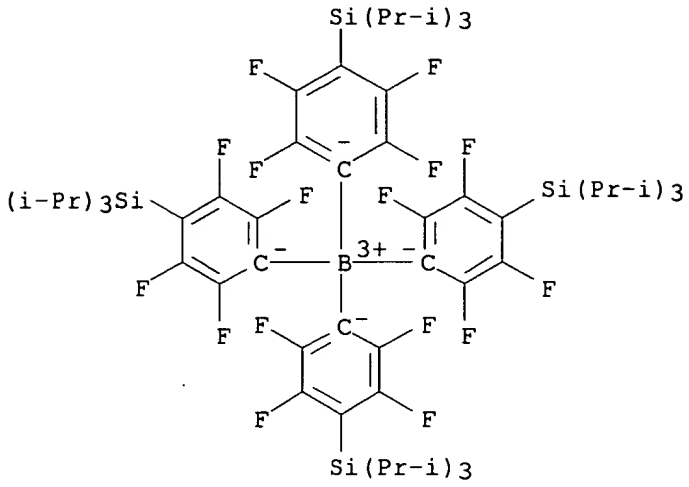


RN 167172-34-1 HCAPLUS
CN Zirconium(1+), hydrobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, tetrakis[2,3,5,6-tetrafluoro-4-[tris(1-

methylethyl)silyl]phenyl]borate(1-) (9CI) (CA INDEX NAME)

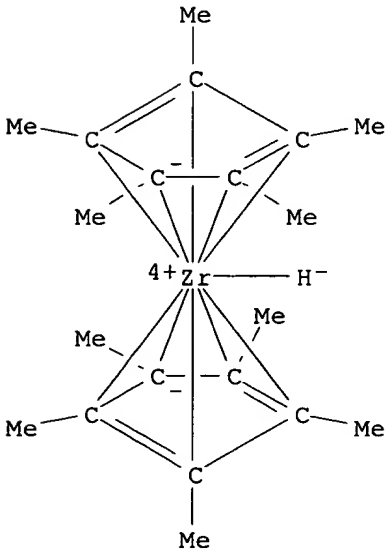
CM 1

CRN 167172-27-2
CMF C60 H84 B F16 Si4
CCI CCS



CM 2

CRN 143565-16-6
CMF C20 H31 Zr
CCI CCS

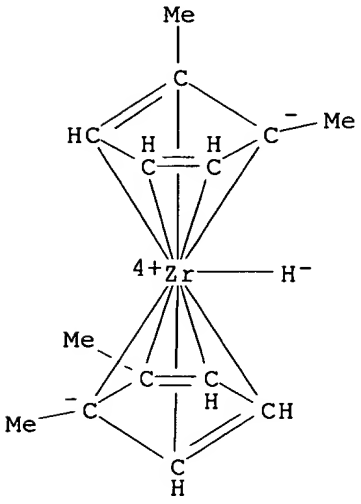


RN 185855-35-0 HCAPLUS

CN Zirconium(1+), bis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]hydro-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

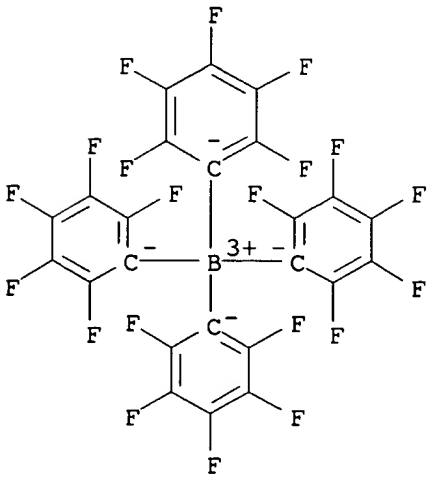
CM 1

CRN 185855-34-9
CMF C14 H19 Zr
CCI CCS



CM 2

CRN 47855-94-7
CMF C24 B F20
CCI CCS

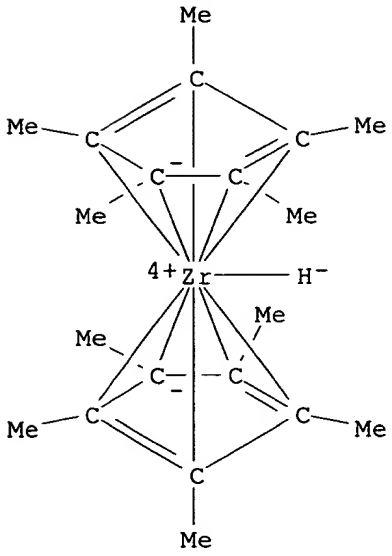


RN 185855-36-1 HCAPLUS
CN Zirconium(1+), hydrobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-

cyclopentadien-1-yl]-, tetrakis(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

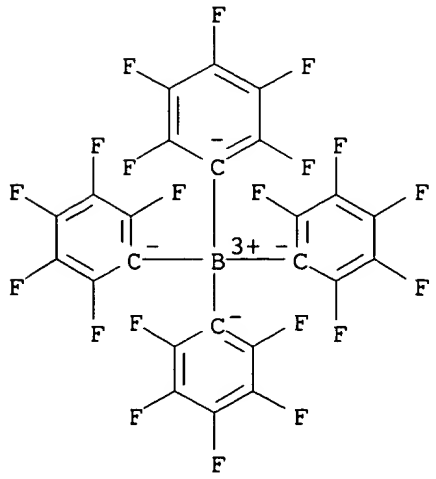
CM 1

CRN 143565-16-6
CMF C20 H31 Zr
CCI CCS



CM 2

CRN 47855-94-7
CMF C24 B F20
CCI CCS



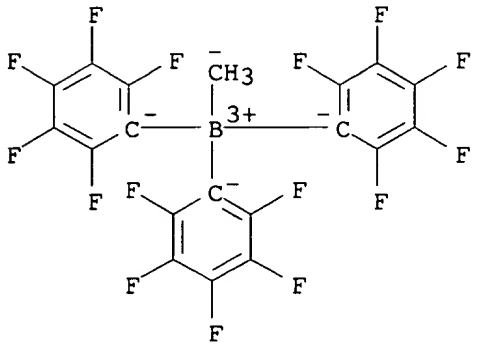
IT **133445-49-5**, Bis(η5-cyclopentadienyl)(methyl)zirconium(1+) methyltris(pentafluorophenyl)borate(1-) **133445-51-9**, Bis(η5-1,2-dimethylcyclopentadienyl)(methyl)zirconium(1+) methyltris(pentafluorophenyl)borate(1-) **133445-52-0**, Methylbis(η5-pentamethylcyclopentadienyl)zirconium(1+) methyltris(pentafluorophenyl)borate(1-)
RL: **CAT (Catalyst use)**; USES (Uses)
(propylene **polymerization** in presence of)

RN 133445-49-5 HCAPLUS

CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

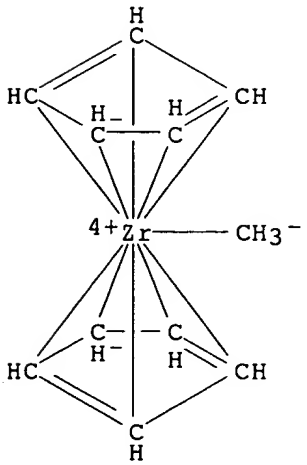
CM 1

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



CM 2

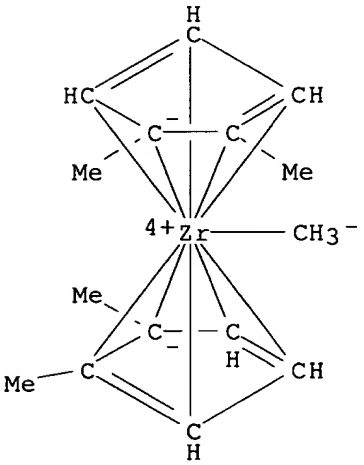
CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS



RN 133445-51-9 HCAPLUS
CN Zirconium(1+), bis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]methyl-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

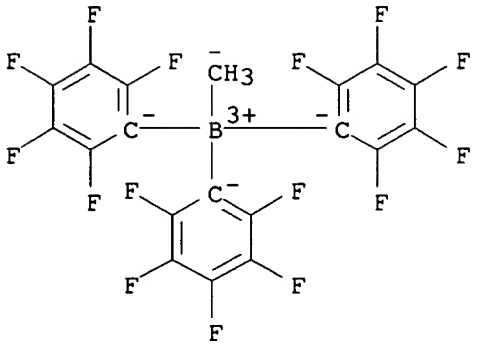
CM 1

CRN 133445-50-8
CMF C15 H21 Zr
CCI CCS



CM 2

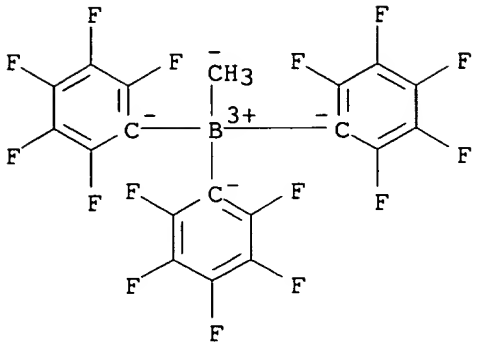
CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



RN 133445-52-0 HCAPLUS
CN Zirconium(1+), methylbis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

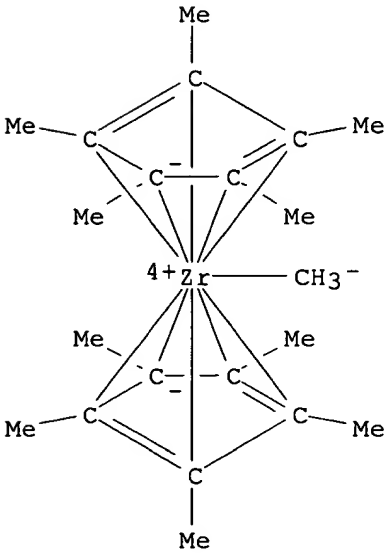
CM 1

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



CM 2

CRN 118611-11-3
CMF C21 H33 Zr
CCI CCS



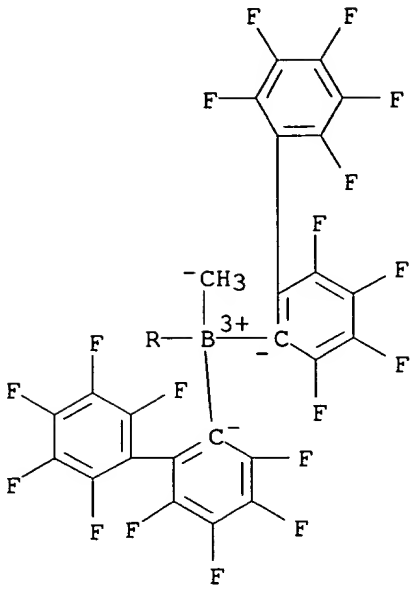
L34 ANSWER 22 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1996:689346 HCAPLUS
DN 126:31699
ED Entered STN: 23 Nov 1996
TI Organo-Lewis Acids As Cocatalysts in Cationic Metallocene Polymerization Catalysis. Unusual Characteristics of Sterically Encumbered Tris(perfluorobiphenyl)borane

AU Chen, You-Xian; Stern, Charlotte L.; Yang, Shengtian; Marks, Tobin J.
CS Department of Chemistry, Northwestern University, Evanston, IL, 60208-3113, USA
SO Journal of the American Chemical Society (1996), 118(49), 12451-12452
CODEN: JACSAT; ISSN: 0002-7863
PB American Chemical Society
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 75
AB The unusual cocatalytic characteristics of sterically hindered tris(perfluoro-2-biphenylyl)borane with metallocenes in olefin polymerization are reported. The characteristics include substantially different abstractive and ion pair structure-reactivity relationships as compared with tris(perfluorophenyl)borane.
ST perfluorobiphenylylborane metallocene catalyst olefin polymn
IT **Crystal** structure
(metallocene/perfluoro-2-biphenylyl)borane catalyst for olefin polymerization)
IT Polymerization catalysts
(metallocene/perfluoro-2-biphenylyl)borane catalyst system for olefin polymerization)
IT **184675-07-8P 184675-10-3P 184675-12-5P**
184675-14-7P 184675-17-0P 184675-19-2P 184686-71-3P
184686-73-5P 184686-74-6P 184686-77-9P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and catalytic properties in olefin **polymerization**)
IT 9002-88-4P, Polyethylene 9003-53-6P, Polystyrene 25213-02-9P, Ethylene-1-hexene copolymer
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation using metallocene/perfluoro-2-biphenylyl)borane catalyst system)
IT **184675-07-8P 184675-10-3P 184675-12-5P**
184686-73-5P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation and catalytic properties in olefin **polymerization**)
RN 184675-07-8 HCAPLUS
CN Zirconium(1+), chlorobis(η5-2,4-cyclopentadien-1-yl)-, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

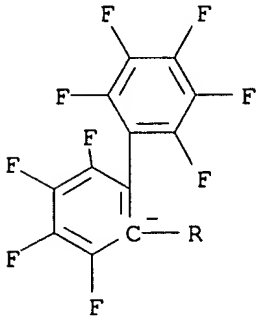
CM 1

CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

PAGE 1-A

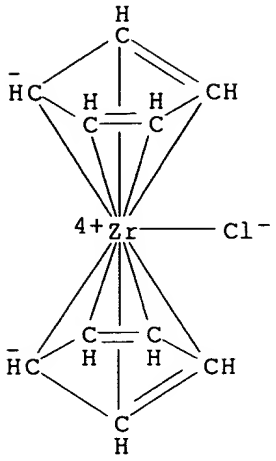


PAGE 2-A



CM 2

CRN 184675-06-7
CMF C10 H10 Cl Zr
CCI CCS

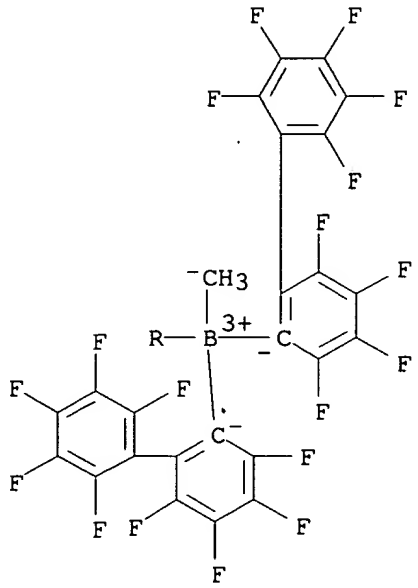


RN 184675-10-3 HCAPLUS
CN Zirconium(1+), tetrakis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]-μ-methyldimethyldi-, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

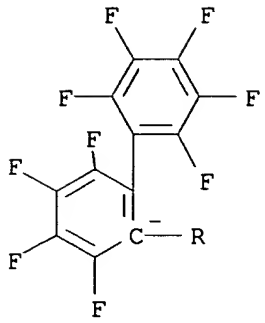
CM 1

CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

PAGE 1-A

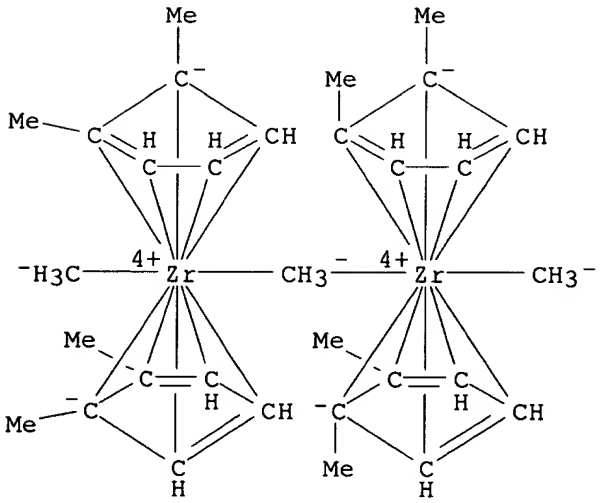


PAGE 2-A



CM 2

CRN 184675-09-0
CMF C31 H45 Zr2
CCI CCS

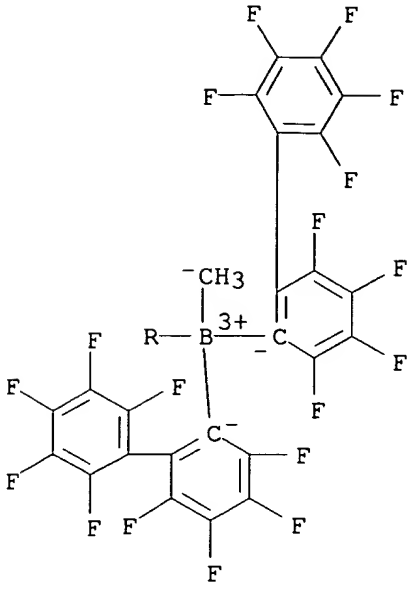


RN 184675-12-5 HCAPLUS
CN Zirconium(1+), μ-methyldimethyltetrakis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]di-, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

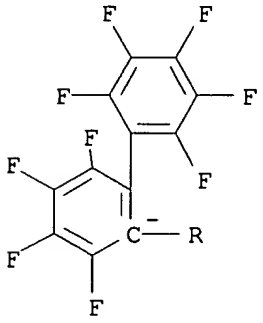
CM 1

CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

PAGE 1-A

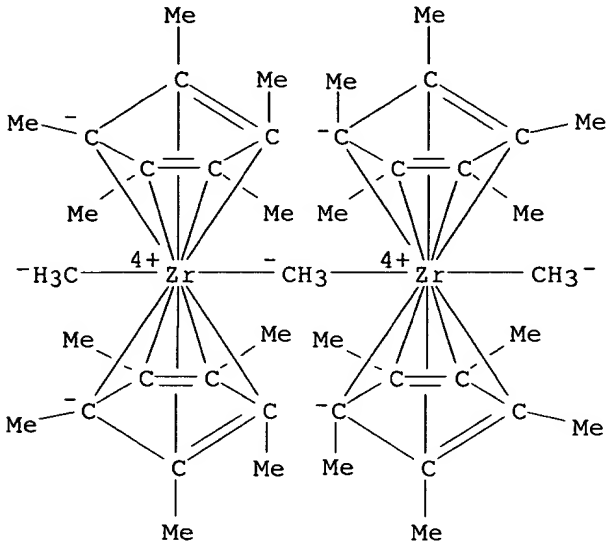


PAGE 2-A



CM 2

CRN 184675-11-4
CMF C43 H69 Zr2
CCI CCS

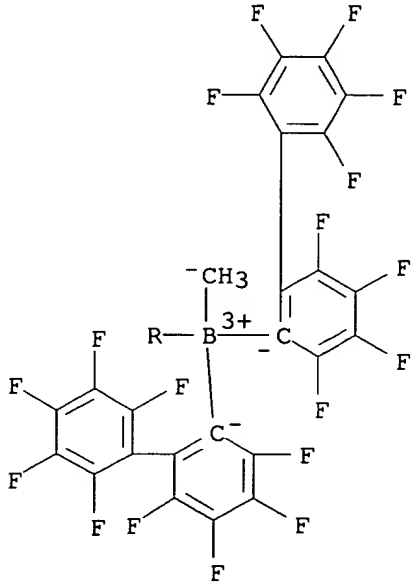


RN 184686-73-5 HCAPLUS
CN Zirconium(1+), tetrakis(η5-2,4-cyclopentadien-1-yl)-μ-methyldimethyldi-, (T-4)-methyltris(2',3,3',4,4',5,5',6,6'-nonafluoro[1,1'-biphenyl]-2-yl)borate(1-) (9CI) (CA INDEX NAME)

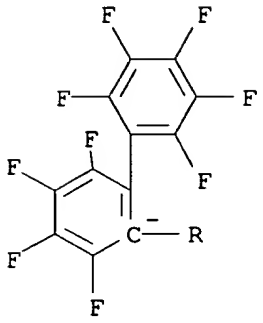
CM 1

CRN 184686-70-2
CMF C37 H3 B F27
CCI CCS

PAGE 1-A

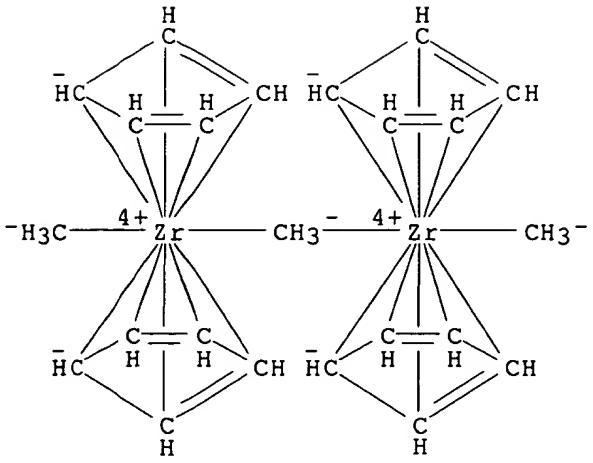


PAGE 2-A



CM 2

CRN 174577-52-7
CMF C23 H29 Zr2
CCI CCS

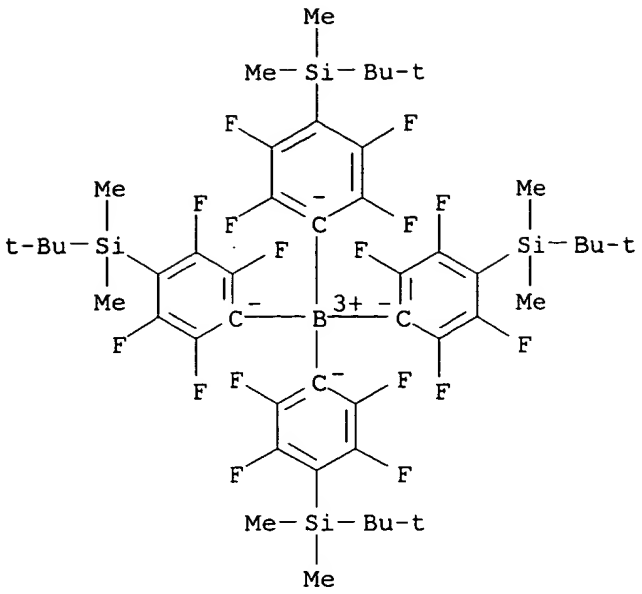


L34 ANSWER 23 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1995:643165 HCAPLUS
DN 123:169780
ED Entered STN: 28 Jun 1995
TI Protected (Fluoroaryl)borates as Effective Counteranions for Cationic Metallocene Polymerization Catalysts
AU Jia, Li; Yang, Xinmin; Ishihara, Atsushi; Marks, Tobin J.
CS Department of Chemistry, Northwestern University, Evanston, IL, 60208-3113, USA
SO Organometallics (1995), 14(7), 3135-7
CODEN: ORGND7; ISSN: 0276-7333
PB American Chemical Society
DT Journal

LA English
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 35
OS CASREACT 123:169780
AB The functionalized (fluoroaryl)borate salts Ph3C+B(C6F4TBS)4- and Ph3C+B(C6F4TIPS)4- (TBS = tBuMe2Si; TIPS = iPr3Si) are prepared in three steps from 1,4-HC6F4Br. Reaction with zirconocene dimethyls yields **crystalline**, thermally stable, soluble L2ZrCH3+B(C6F4SiR3)4- and L'2ZrH+B(C6F4SiR3)4- salts (L = η5-C5H5; η5-1,2-Me2C5H3; L' = Me5C5) which function as highly active ethylene polymerization catalysts.
ST fluoroaryl borate prepn reaction zirconocene dimethyl; polymn catalyst zirconocene fluoroaryl borate prepn
IT Polymerization catalysts
(preparation of protected (fluoroaryl)borates as effective counter anions for cationic metallocene polymerization catalysts)
IT **167172-29-4P 167172-30-7P 167172-31-8P**
167172-32-9P 167172-33-0P 167172-34-1P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of protected (fluoroaryl)borates as effective counter anions for cationic metallocene **polymerization** catalysts)
IT 74-85-1, Ethene, reactions 1559-88-2, 1-Bromo-2,3,5,6-tetrafluorobenzene 10294-34-5, Boron trichloride 12636-72-5, Dimethylzirconocene 67108-80-9 69739-34-0, tert-Butyldimethylsilyl trifluoromethanesulfonate 80522-42-5 106865-92-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of protected (fluoroaryl)borates as effective counter anions for cationic metallocene polymerization catalysts)
IT 167172-21-6P 167172-22-7P 167172-23-8P 167172-24-9P 167172-26-1P 167172-28-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of protected (fluoroaryl)borates as effective counter anions for cationic metallocene polymerization catalysts)
IT **167172-29-4P 167172-30-7P 167172-31-8P**
167172-32-9P 167172-33-0P 167172-34-1P
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of protected (fluoroaryl)borates as effective counter anions for cationic metallocene **polymerization** catalysts)
RN 167172-29-4 HCAPLUS
CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, tetrakis[4-[(1,1-dimethylethyl)dimethylsilyl]-2,3,5,6-tetrafluorophenyl]borate(1-) (9CI) (CA INDEX NAME)

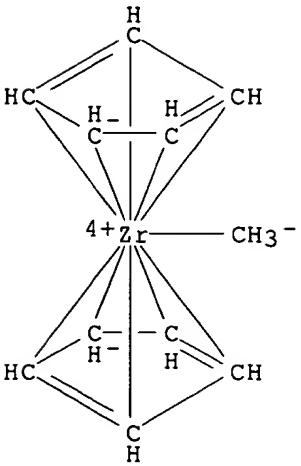
CM 1

CRN 167172-25-0
CMF C48 H60 B F16 Si4
CCI CCS



CM 2

CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS

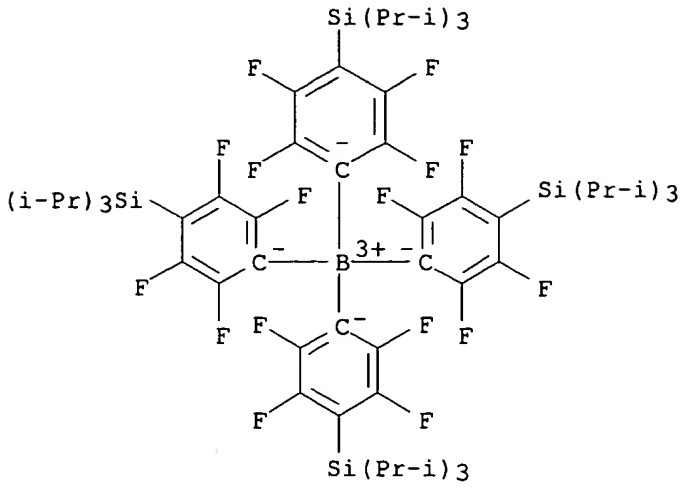


RN 167172-30-7 HCAPLUS
CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, tetrakis[2,3,5,6-tetrafluoro-4-[tris(1-methylethyl)silyl]phenyl]borate(1-) (9CI) (CA INDEX NAME)

CM 1

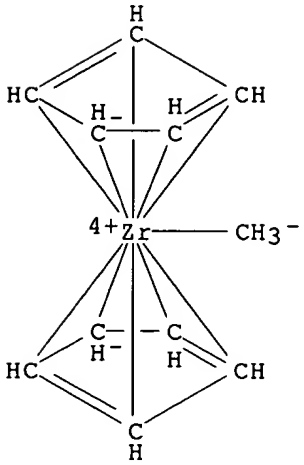
CRN 167172-27-2

CMF C60 H84 B F16 Si4
CCI CCS



CM 2

CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS

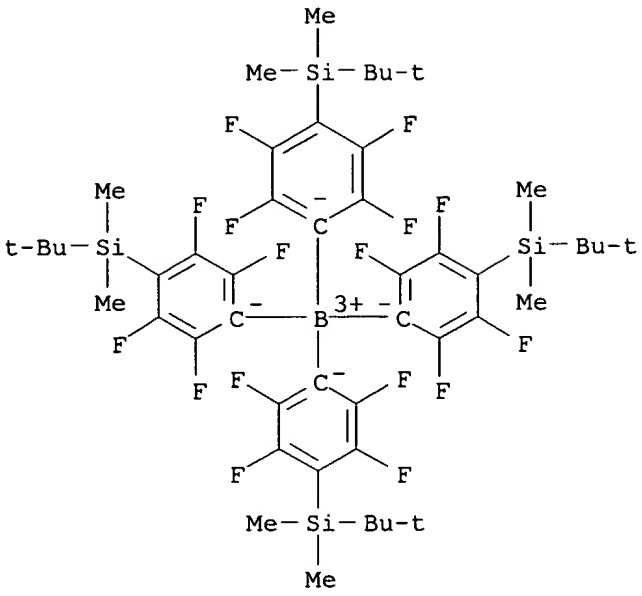


RN 167172-31-8 HCAPLUS
CN Zirconium(1+), bis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]methyl-, tetrakis[4-[(1,1-dimethylethyl)dimethylsilyl]-2,3,5,6-tetrafluorophenyl]borate(1-) (9CI) (CA INDEX NAME)

CM 1

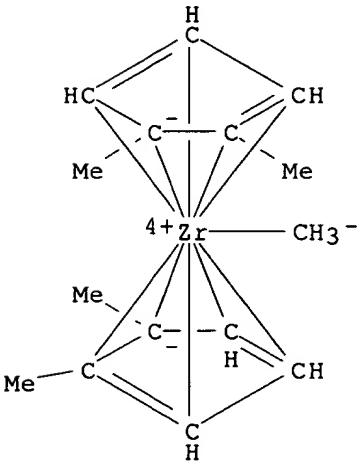
CRN 167172-25-0
CMF C48 H60 B F16 Si4

CCI CCS



CM 2

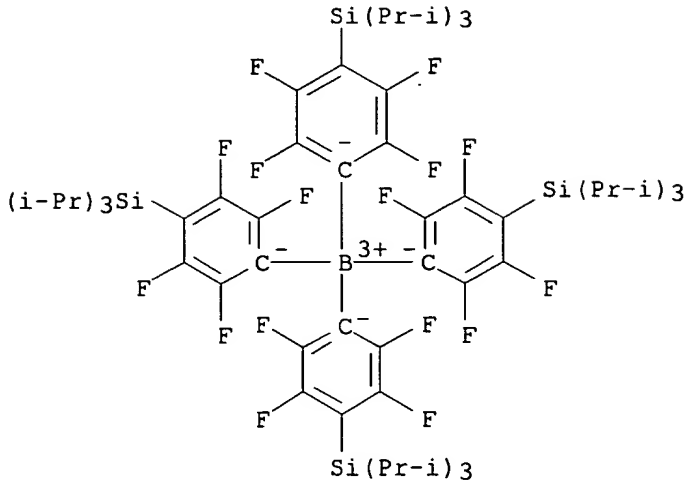
CRN 133445-50-8
CMF C15 H21 Zr
CCI CCS



RN 167172-32-9 HCAPLUS
CN Zirconium(1+), bis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]methyl-, tetrakis[2,3,5,6-tetrafluoro-4-[tris(1-methylethyl)silyl]phenyl]borate(1-) (9CI) (CA INDEX NAME)

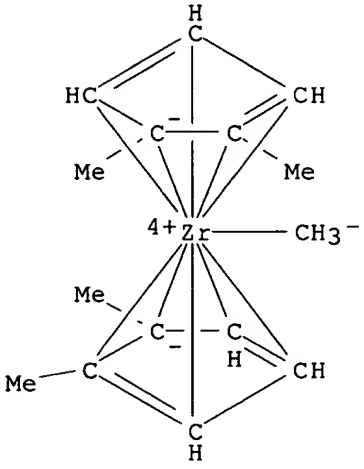
CM 1

CRN 167172-27-2
CMF C60 H84 B F16 Si4
CCI CCS



CM 2

CRN 133445-50-8
CMF C15 H21 Zr
CCI CCS



RN 167172-33-0 HCAPLUS
CN Zirconium(1+), hydrobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, tetrakis[4-[(1,1-dimethylethyl)dimethylsilyl]-2,3,5,6-tetrafluorophenyl]borate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 167172-25-0
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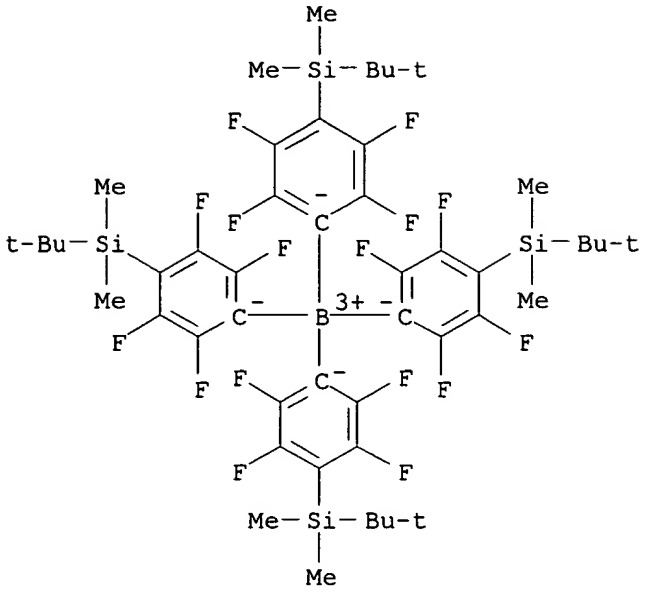
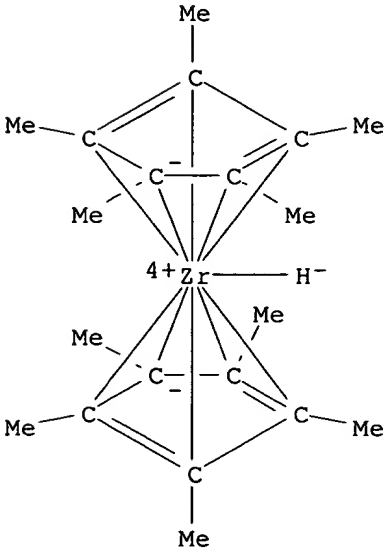
CCI CCS



CM 2

CRN 143565-16-6
CMF C20 H31 Zr
CCI CCS

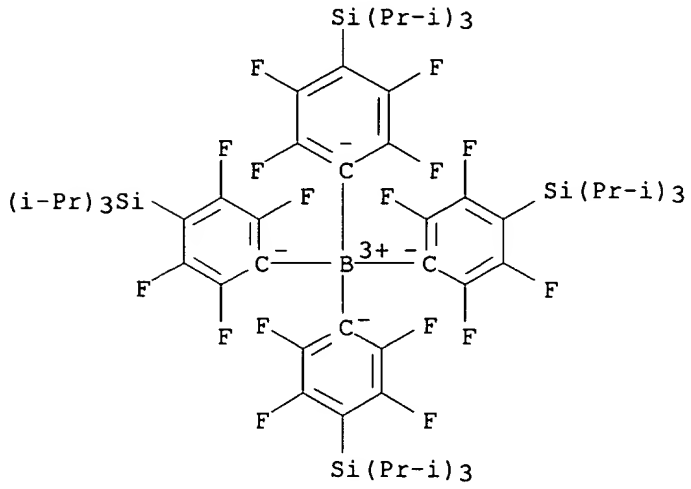


RN 167172-34-1 HCAPLUS

CN Zirconium(1+), hydrobis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, tetrakis[2,3,5,6-tetrafluoro-4-[tris(1-methylethyl)silyl]phenyl]borate(1-) (9CI) (CA INDEX NAME)

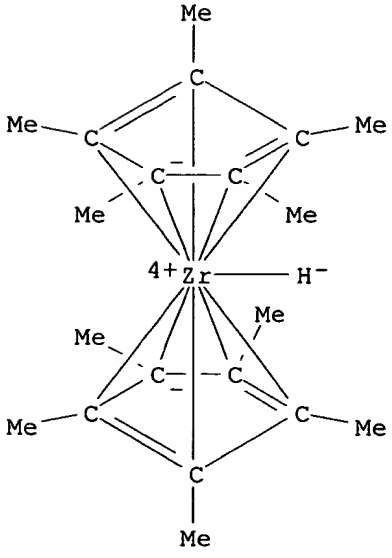
CM 1

CRN 167172-27-2
CMF C60 H84 B F16 Si4
CCI CCS



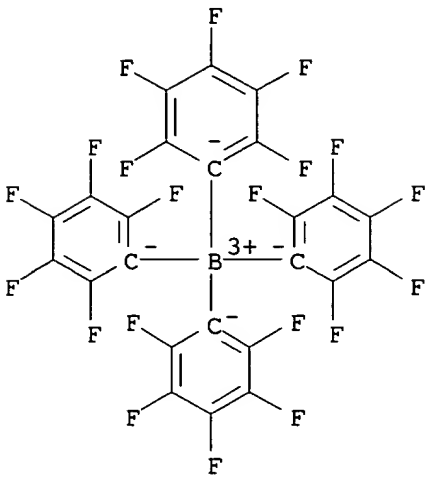
CM 2

CRN 143565-16-6
CMF C20 H31 Zr
CCI CCS



CM 2

CRN 47855-94-7
CMF C24 B F20
CCI CCS

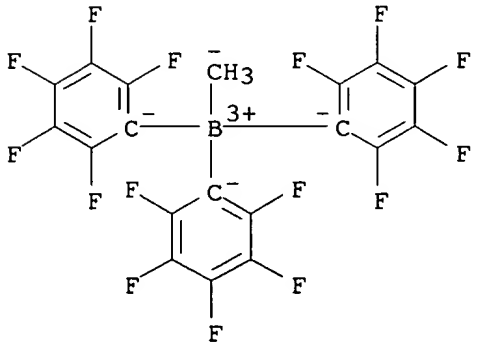


L34 ANSWER 26 OF 26 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:186158 HCAPLUS
DN 114:186158
ED Entered STN: 17 May 1991
TI Cation-like homogeneous olefin polymerization catalysts based upon zirconocene alkyls and tris(pentafluorophenyl)borane
AU Yang, Xinmin; Stern, Charlotte L.; Marks, Tobin J.
CS Dep. Chem., Northwestern Univ., Evanston, IL, 60208, USA
SO Journal of the American Chemical Society (1991), 113(9), 3623-5
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA English
CC 35-3 (Chemistry of Synthetic High Polymers)
AB The reaction of zirconocene dialkyls L2ZrMe2 (L = η5-C5H5, η5-1,2-Me2C5H3, η5-C5Me5) with B(C6F5)3 yields "cation-like" zirconocene complexes L2ZrMe+MeB(C6F5)3-. (1,2-Me2C5H3)2ZrMe+MeB(C6F5)3- was characterized **crystallog**. With the exception of a shortened Zr-Me distance [2.252(4) Å], the metrical parameters within the "bent sandwich" L2ZrMe+ cation are unexceptional. The cation interacts weakly via a highly unsym. Zr-(μ-Me)B bridge with the essentially tetrahedral MeB(C6F5)3- anion. The L2ZrMe+MeB(C6F5)3- complexes are active catalysts for olefin polymerization For ethylene polymerization, Nt(1) ≈ 45 s-1 at 25°, 1 atm (.apprx.4.5 + 106 g polyethylene/mol Zr h atm) to yield linear polyethylene. For propylene polymn at 25°, 1-5 atm, atactic polypropylene is produced with Nt(1) ≈ 4.2 s-1.
ST zirconocene complex catalyst polymn olefin; ethylene polymn zirconocene complex catalyst; propylene polymn zirconocene complex catalyst; **crystal** structure zirconocene complex catalyst
IT **Crystal** structure
(of zirconocene complex catalyst for polymerization of ethylene or propylene)

IT Polymerization catalysts
(zirconocene complexes, for ethylene or propylene)
IT **133445-49-5 133445-52-0**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for olefin **polymerization**)
IT **133445-51-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for olefin **polymerization**, **crystal** structure of)
IT 9002-88-4P, Polyethylene 9003-07-0P, Atactic polypropylene
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in presence of cationlike zirconocene complexes)
IT **133445-49-5 133445-52-0**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for olefin **polymerization**)
RN 133445-49-5 HCAPLUS
CN Zirconium(1+), bis(η5-2,4-cyclopentadien-1-yl)methyl-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

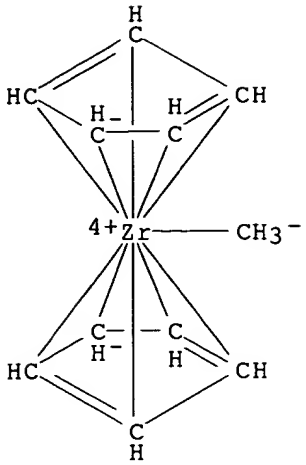
CM 1

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



CM 2

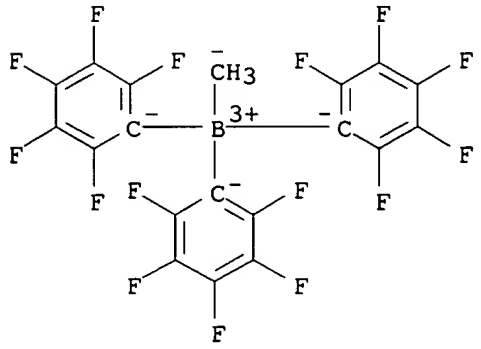
CRN 94370-49-7
CMF C11 H13 Zr
CCI CCS



RN 133445-52-0 HCAPLUS
CN Zirconium(1+), methylbis[(1,2,3,4,5-η)-1,2,3,4,5-pentamethyl-2,4-cyclopentadien-1-yl]-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

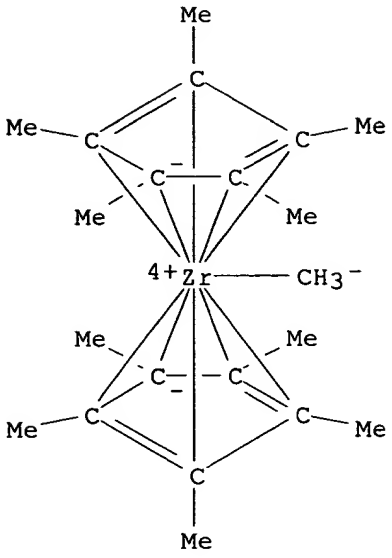
CM 1

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



CM 2

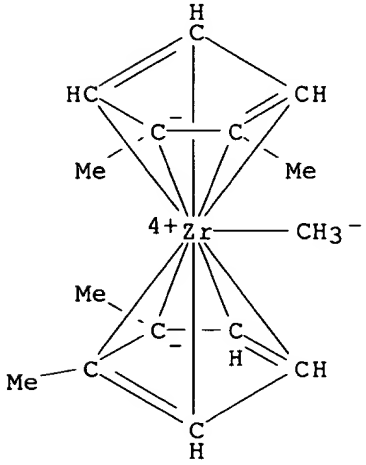
CRN 118611-11-3
CMF C21 H33 Zr
CCI CCS



IT **133445-51-9**
RL: **CAT (Catalyst use)**; USES (Uses)
(catalysts, for olefin **polymerization**, **crystal** structure of)
RN 133445-51-9 HCAPLUS
CN Zirconium(1+), bis[(1,2,3,4,5-η)-1,2-dimethyl-2,4-cyclopentadien-1-yl]methyl-, (T-4)-methyltris(pentafluorophenyl)borate(1-) (9CI) (CA INDEX NAME)

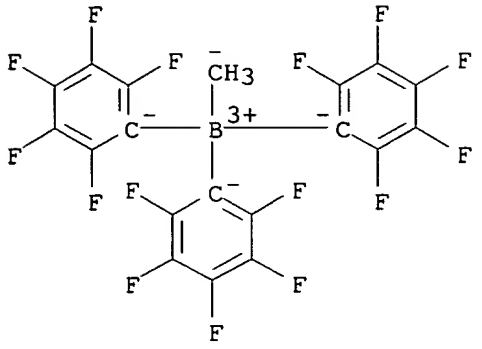
CM 1

CRN 133445-50-8
CMF C15 H21 Zr
CCI CCS



CM 2

CRN 133445-48-4
CMF C19 H3 B F15
CCI CCS



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